Committee for Risk Assessment (RAC)
Committee for Socio-economic Analysis (SEAC)

Background document
to the Opinions on the Annex XV dossier proposing restrictions on five
Phenylmercury compounds

ECHA/RAC/RES-O-0000001362-83-02/S1
ECHA/SEAC/[reference code to be added after the adoption of the SEAC opinion]

SUBSTANCE NAME	IUPAC NAME	EC NUMBER	CAS NUMBER
Phenylmercury acetate	Phenylmercury acetate	200-532-5	62-38-4
Phenylmercury propionate	Phenylmercury propionate	203-094-3	103-27-5
Phenylmercury 2-ethylhexanoate	Phenylmercury 2-ethylhexanoate	236-326-7	13302-00-6
Phenylmercury octanoate	Phenylmercury octanoate	-	13864-38-5
Phenylmercury neodecanoate	Phenylmercury neodecanoate	247-783-7	26545-49-3

This Background Document (BD) shall be regarded as further reference material to the opinions of the Committees for Risk Assessment and Socio-economic Analysis. It contains further details and assessment in addition/beyond the justifications provided in the opinions including, where relevant, information that has been received during the opinion making process and may be used to better understand the opinions and their justifications. The BD is a supporting document based on the Annex XV restriction report submitted by MS, and updated to support the opinions of the Committees.

4 July 2011

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Preface

Mercury and its compounds are highly toxic to humans, ecosystems and wildlife. A key aim of the Community Strategy Concerning Mercury (European Commission, 2005) is to reduce mercury levels in the environment and to reduce human exposure. The European Community has already taken a range of measures to reduce mercury emissions and uses, but still more remains to be done. An assessment of options for reducing major inputs of mercury to society identified the use of phenylmercury compounds as catalysts in polyurethane systems as a significant source (Cowi and Concorde East/West, 2008). We propose to restrict the manufacture and use of these substances to reduce the overall input of mercury to the environment and hence to reduce the impact of mercury on health and environment in Europe and globally.

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A PROPOSAL

A.1 Proposed restrictions

A.1.1 The identity of the substances

Substance name	**Phenylmercury acetate**
IUPAC name	Phenylmercury acetate
EC number	200-532-5
CAS number	62-38-4

Substance name	**Phenylmercury propionate**
IUPAC name	Phenylmercury propionate
EC number	203-094-3
CAS number	103-27-5

Substance name	**Phenylmercury 2-ethylhexanoate**
IUPAC name	Phenylmercury 2-ethylhexanoate
EC number	236-326-7
CAS number	13302-00-6

Substance name	**Phenylmercury octanoate**
IUPAC name	Phenylmercury octanoate
EC number	-
CAS number	13864-38-5

Substance name	**Phenylmercury neodecanoate**
IUPAC name	Phenylmercury neodecanoate
EC number	247-783-7
CAS number	26545-49-3

A.1.2 Scope and conditions of restrictions

A.1.2.1 Restriction originally proposed in the Annex XV dossier by the dossier submitter

Phenylmercury acetate (CAS 62-38-4, EC 200-532-5)
Phenylmercury propionate (CAS No 103-27-5, EC No 203-094-3)
Phenylmercury 2-ethylhexanoate (CAS No 13302-00-6, EC No 236-326-7)
Phenylmercuric octanoate, (CAS No 13864-38-5, EC No na*)
Phenylmercury neodecanoate (CAS No 26545-49-3, EC No 247-783-7)

1. Shall not be manufactured, placed on the market, or used, as a substance or in mixtures in a concentration above 0.01 % Hg weight by weight (w/w) after [5 years of the entry into force].

2. Articles, or homogenous parts of articles, containing the substance(s) in a concentration above 0.01 % Hg weight by weight (w/w) shall not be placed on the market [5 years of the entry into force].

A.1.2.2 Restriction proposed in the first version of the background document

In order to make the wording more similar to the restriction under development on dimethylfumarate (DMFu) the dossier submitter reworded the restriction proposal in the first version of the background document. The changes also aimed to take into account comments in the first FORUM advice saying that the dossier did not provide clarity on how the qualitative and quantitative determination of a phenylmercury compound has to be done. As a consequence, FORUM thought control of compliance with the limit value seemed difficult.

Phenylmercury acetate (CAS 62-38-4, EC 200-532-5)
Phenylmercury propionate (CAS No 103-27-5, EC No 203-094-3)
Phenylmercury 2-ethylhexanoate (CAS No 13302-00-6, EC No 236-326-7)
Phenylmercuric octanoate, (CAS No 13864-38-5, EC No na*)
Phenylmercury neodecanoate (CAS No 26545-49-3, EC No 247-783-7)

1. Shall not be manufactured, placed on the market, or used, as a substance or in mixtures after [5 years of the entry into force].

2. Articles, or parts of articles, containing the substance(s) shall not be placed on the market after [5 years of the entry into force].

3. The provisions referred to in paragraphs 1 and 2 above concerning mixtures and articles shall be regarded as kept when the concentration in a mixture or in any sample from one article, respectively, does not exceed 0.01 % weight by weight (w/w) mercury.

*Na: not available

A.1.2.3 Restriction proposed in the final adopted RAC opinion

RAC recommended an implementation time of 3 years instead of 5 years in order to further reduce emissions, see section E.2.3. They also adjusted the wording to take the suggestions by FORUM in their second advice into account. Forum suggested to replace "shall be regarded as kept when" by "are not applicable if" to make the text more clear. As in the case of the DMFu restriction, they also considered the wording "any parts thereof" as preferable to the original one since, for Annex XVII restrictions, the use of "any parts thereof" could be regarded as guidance for sampling.

Phenylmercury acetate (CAS 62-38-4, EC 200-532-5)
Phenylmercury propionate (CAS No 103-27-5, EC No 203-094-3)
Phenylmercury 2-ethylhexanoate (CAS No 13302-00-6, EC No 236-326-7)
Phenylmercuric octanoate, (CAS No 13864-38-5, EC No na*)
Phenylmercury neodecanoate (CAS No 26545-49-3, EC No 247-783-7)

1. Shall not be manufactured, placed on the market, or used, as a substance or in mixtures after 3 years of the entry into force*.

2. Articles, or parts of articles, containing the substance(s) shall not be placed on the market after 3 years of the entry into force*.

*The provisions referred to in paragraphs 1 and 2 above concerning mixtures and articles are not applicable if the concentration in a mixture or in articles or any parts thereof does not exceed 0.01 % weight by weight (w/w) mercury.

In addition to the proposed restriction RAC also added to their final opinion an important consideration regarding the restriction;
RAC considers that if the five substances mentioned above were to be replaced by other organomercury compounds** this restriction could become ineffective. Therefore, in addition to the conditions mentioned above, RAC recommends considering necessary measures for verifying and controlling that other organomercury compounds are not used as alternative to the restricted substances.

**Other organomercury compounds that may be used as catalysts in the polymer production and have the general formula (R-Hg)*n*-X where wherein R is aryl, aralkyl, alkaryl, heterocyclic or straight, branched alkyl, or cyclic lower alkyl; and the halo, amido, carboxy, lower alkoxy or nitro substituted derivatives thereof, X is an saturated or unsaturated, branched, straight or aromatic carboxylate, and *n* is an integer of 1-4.

A.1.2.4 Restriction proposed in the agreed SEAC draft opinion

SEAC kept the 5 year implementation period, as proposed by the dossier submitter. Apart from this, the wording of the recommended restriction is similar to the one in the final RAC opinion.

Phenylmercury acetate (CAS 62-38-4, EC 200-532-5)

Phenylmercury propionate (CAS No 103-27-5, EC No 203-094-3)
Phenylmercury 2-ethylhexanoate (CAS No 13302-00-6, EC No 236-326-7)
Phenylmercuric octanoate, (CAS No 13864-38-5, EC No na*)
Phenylmercury neodecanoate (CAS No 26545-49-3, EC No 247-783-7)

1. Shall not be manufactured, placed on the market, or used, as a substance or in mixtures after 5 years of the entry into force.

2. Articles, or parts of articles, containing the substance(s) shall not be placed on the market after 5 years of the entry into force.

The provisions referred to in paragraphs 1 and 2 above concerning mixtures and articles are not applicable if the concentration in a mixture or in articles or any parts thereof does not exceed 0.01 % weight by weight (w/w) mercury.

*Na: not available

A.2 Summary of the justification

A.2.1 Identified hazard and risk

Main concerns related to mercury and mercury compounds and actions at a regional and global level
Mercury and its compounds are highly toxic to humans, ecosystems and wildlife, in particular when chemically converted to methylmercury. The nervous system and the developing brain are thought to be the most sensitive target organs. A complete discussion on the risks of mercury and mercury compounds is beyond the scope of this report.

Mercury is found both naturally and as an introduced contaminant in the environment. Anthropogenic emissions have widespread impacts on human and environmental health. Mercury is considered to be a global persistent pollutant; in the environment it cannot be broken down to any harmless form. Once emitted, mercury enters the complex biogeochemical cycle. After intensive use of mercury over many years mercury can be found in almost all environmental compartments, like the atmosphere, soil and water systems and in biota all over the world. The formation of methylmercury and subsequent biomagnification in food chains are of serious concern. It is necessary to reduce the risk of exposure to mercury for humans and the environment. The key, long term benefit of reducing mercury emissions will be decreased levels of mercury in the environment. This, in turn, will lead to lower levels of human exposure to mercury, including methylmercury in fish, with resultant health benefits. It will also reduce the impacts of mercury on soils and biodiversity.

According to EFSA the estimated intake of mercury from food (in the form of methylmercury) in Europe varies between countries, depending on the amount and the type of fish consumed. The mean intakes were in most cases below the JECFA[1] PTWI[2] of 1.6 µg/kg

[1] The FAO/ WHO Joint Expert Committee on Food Additives (JECFA)

body weight but high intakes may exceed it. Children seem to be more likely to exceed the PTWI than adults. In Norway and Sweden a significant increase of mercury levels in certain freshwater fish species has been observed during the last decade. The EU maximum level of 0.5 mg Hg/kg wet weight (related to placing on the market of foodstuff) is exceeded in many cases. Concerning indirect exposure of man via the environment the level of methylmercury in fish, and in particular the data indicating increasing levels in the last 10 years in some areas, is of serious concern. It is not known if the increase in levels in freshwater fish is a general trend for Europe.

Once released into the atmosphere, mercury can undergo long-range atmospheric transport, hence the atmosphere is the most important pathway for the worldwide dispersion and transport of mercury in the environment. The Arctic is believed to be a global sink of mercury due to a set of extraordinary circumstances occurring during Polar spring. Certain indigenous communities, for example in the Arctic, have been shown to be particularly vulnerable due to high levels of deposition and accumulation of methylmercury in their traditional foods (even though they use and emit virtually no mercury).

The global threat from mercury releases warrants action at local, national, regional and global level. There is now a world-wide common effort to reduce both demand and supply of mercury. In 2009, the UN Environment Governing Council agreed to take steps towards a global legally binding instrument to control uses and emissions of mercury. The Council of the European Union supports this step towards an international treaty.

The European Union has made considerable progress in addressing the global challenges of mercury since it launched the EU mercury strategy in 2005. This has resulted in restrictions on the placing on the market of measuring devices containing mercury, a ban on exports of mercury from the EU that will come into force in 2011 and new rules on safe storage. The EU's mercury strategy is a comprehensive plan addressing mercury pollution both in the EU and globally. It contains 20 measures to reduce mercury emissions, cut supply and demand and protect against exposure, especially to methylmercury found in fish.

The EU mercury strategy action 8 specifies that the Commission will further study in the short term the few remaining products and applications in the EU that use small amounts of mercury. In the medium to longer term, any remaining uses may be subject to limitations under the REACH regulation. According to action 10 the Commission will undertake further study in the short to medium term of the fate of mercury products already circulating in society.

The report "Options for reducing mercury use in products and applications and the fate of mercury already circulating in society" (Cowi and Concorde East/West, 2008) addresses among others actions 8 and 10 in the EU mercury strategy. The aim of the study was to identify the possibilities for further reducing mercury use in products and applications and for reducing the amounts of mercury already in society. The study gives an overview on the situation in the EU-27, Norway and Switzerland and quantifies the mercury use for some significant applications of mercury that have drawn less attention until now, including the uses of certain phenylmercury compounds as catalysts in polyurethane systems. The purpose of this Annex XV dossier has been to further investigate this particular source of mercury emissions and the possibility for restrictions on the manufacture and use of these compounds.

[2] Provisional Tolerable Weekly Intake

The arguments for taking action to address the risks from these substances relates to their contribution to the general and wider/global mercury problem, which the EU mercury strategy and the UNEP global mercury program serves to highlight. The justification for action can be put in the context of a widely recognized need to further reduce mercury emissions at an EU and global level.

Risk assessment of the phenylmercury compounds

Based on the information obtained (Section B.2) it is estimated that around 130-260 tpa of phenylmercury catalysts are manufactured in Europe, however 55-110 tpa are manufactured exclusively for export. So only 75 – 150 tpa of phenylmercury compounds are manufactured for use in the production of phenylmercury catalysts in EU+EFTA, of which 40 – 85 tpa are exported. Finally, around 36 – 70 tpa of phenylmercury compounds in catalysts (i.e. 16 – 31.3 tpa mercury, calculated from the mercury/phenylmercury-neodecanoate ratio) are used per annum in the EU+EFTA, this includes a minor import.

There are a number of applications for phenylmercury-catalysed polyurethanes (Section B.2), for example in gaskets and seals, encapsulant for electronic assemblies, film and television props, vibration dampers, clear PU on labels, water resistant coatings and concrete sealants, marine repair and repair on conveyor belts, rollers on swivel chairs and roller skates and in shoe soles. They have also been used in floorings, but current use has not been confirmed.

The assessment of the five phenylmercury compounds is mainly based on data for phenylmercury acetate since most information is available for this substance (Section B.3-B.11). Due to the fact that the phenylmercury compounds are degraded in the environment to give hazardous degradation products, i.e. inorganic mercury and elemental mercury, which can be transformed to methylmercury (Section B.4), the risk assessment should give consideration to the risks that might arise from the degradation/transformation products as well.

PBT assessment

The RAC assessment is presented in detail in the RAC opinion. The assessment presented by the dossier submitter (Norway) is reproduced below for transparency.

Phenylmercury compounds
A summary with available test data and calculated data for the five phenylmercury compounds in relation to PBT criteria is compiled in Section B.8.1.4. According to the EU classification of phenlmercury acetate (T, R48 and STOT RE 1, H372) and of the other phenylmercury compounds (STOT RE 2), phenylmercury acetate, phenylmercury propionate, (2-ethylhexanoato) phenylmercury, phenylmercury octanoate and phenylmercury neodecanoate fulfil the T criterion in REACH Annex XIII.
All five phenylmercury compounds dissociate rapidly into phenylmercury cation and carboxylate anion followed by a rapid hydrolysis of phenylmercury to phenylmercury hydroxide. With phenylmercury as the common intermediate, it is considered likely that the propionate, octanoate, 2-ethylhexanoate and neodecanoate do not behave differently from the phenylmercury acetate with regard to biodegradation. Half-lives for phenylmercury acetate in waters, sediments and soils are below the persistency criterion (P).
Estimated BCFs for the 5 phenylmercury compounds in water at pH5 are between 100 and 1579 and the criterion for bioaccumulation (B) is not fulfilled.

The five phenylmercury compounds themselves are therefore not considered as PBT or vPvB substances.

Degradation/transformation products

Methylmercury:
A summary with available data for methylmercury in relation to the PBT criteria is compiled in Section B.8.1.4.

Persistency:
Concerning the persistency (P) criteria the facts that demethylation occurs at a much lower rate than methylation under certain environmental conditions and that the biological half-life for elimination of methylmercury is high (2 years) should be judged as of equivalent concern. As documented in Section B.4 the release and degradation of the phenylmercury compounds contributes to the pool of elemental and inorganic mercury which cannot be broken down to any harmless form. The cycling of mercury means that the source of methylmercury in the environment is always present once released. The measured environmental concentrations of mercury and methylmercury and the increasing trends of methylmercury levels in biota are of concern.

Bioaccumulation:
The release of the phenylmercury compounds implies a risk of formation of methylmercury. Fish appears to strongly accumulate methylmercury. Most of the methylmercury in fish tissue is covalently bound to protein sulfhydryl groups. This strong binding is the reason for a long half-life of about two years in biota and as a consequence methylmercury is biomagnified significantly through the food web, substantiated by BAF factors in the range from about 20 000 to over 20 000 000. With BCF factors in fish in the range of 8140 up to 85700 methylmercury clearly fulfils the REACH Annex XIII criteria for bioaccumulation (B) and the criteria for very bioaccumulative (vB). According to annex XIII other information on the

bioaccumulation potential such as measured elevated levels in biota can be provided. Detection of elevated mercury levels in fish show that in Scandinavia and North America elevated concentrations of Hg is often found in Northern pike and perch, and the concentrations are often above the limit recommended for human consumption concentrations.

Toxicity:
The criteria for toxicity (T) with a NOEC of 0.26 µg/L for a *Daphnia magna* reproduction test and a provisionally agreed classification of methylmercury as Repr. Cat 1; R61, Repr. Cat 3; R62 and T; R48/25 is clearly fulfilled.

Results from long term or reproductive toxicity testing with birds can be considerd for the assessment of the toxicity property according to annex XIII. Methylmercury is highly toxic to birds described in literature where field observations indicate that in certain fish-eating avian species (divers, sea eagle, fish eagle), intoxications and reproductive impairment were noted after eating fish contaminated with methylmercury at concentrations of 0.2 to 0.7 mg/kg.

Overall, it is concluded that methylmercury is a PBT like substance or a substance of equivalent concern. Methylmercury clearly fulfils the REACH Annex XIII criteria for both bioaccumulation (B) and very bioaccumulative (vB) and for toxicity (T). Concerning the persistency criteria the fact that demethylation occurs at a much lower rate than methylation under certain environmental conditions, and the fact that the biological half-life of methylmercury is high, are of relevance. The cycling of mercury means that the source of methylmercury in the environment is always present once released. The measured environmental concentrations of mercury and methylmercury and the increasing trends of methylmercury levels in biota are of concern.

Substances forming PBT like substances. Qualitative risk assessment (Section B.11.2)
The PBT-assessment shows that degradation/transformation products, i.e. methylmercury, is a PBT like substance. According to REACH, if transformation/degradation products with PBT-properties are being generated, the substances themselves must be treated like PBT-substances with regard to emission estimation and exposure control. To this end, the exposures and emissions to humans and the environment should be minimized to the extent possible.

The use of the catalysts is wide dispersive. Moreover, the mercury catalysts are incorporated into the polymer structure and remain in the final article. The mercury-based products are used both for the professional market and for consumer products. The life-cycle of the substances used in the EU+EFTA is estimated to lead to a release of 6.4 tpa of mercury to the environment (6.1 tpa to air) in 2008. This was estimated at around 4% of the estimated European emissions of mercury in 2005 and at around 7% of the reported emissions to air for EU-27 in 2008. Main releases are assumed to be from formulation and processing (large number of sites) service life and the waste phase. Once emitted, mercury enters the complex biogeochemical cycle.

The potential for formation of methylmercury, that is a PBT like substance, is of major concern and is a main reason for proposing the restrictions.

Quantitative risk assessment (Section B.11.3)

RAC considers that if transformation/degradation products with PBT-properties are being generated, the substances themselves must be treated like PBT-substances with regard to emission estimation and exposure control. For this reason, discussions of risks based on PEC/PNEC considerations in the background document are not of particular relevance to the opinion. The assessment presented by Norway as DS is reproduced below for transparency.

The PBT-assessment concludes that the phenylmercury compounds themselves are not PBT or vPvB-substances and therefore also a quantitative risk assessment approach can be used. However, due to lack of data and also due to the fate of phenylmercury compounds in the environment it is proposed to perform the quantitative risk assessment for environment on the basis of the inorganic mercury data. However, it should be borne in mind that a piece by piece risk assessment of releases of mercury and mercury compounds from single product groups does not give the full picture of the risks, for that purpose different sources of releases would have to be combined. This is considered to be outside the scope of this risk assessment.

The quantitative risk characterisation for consumers indicates that phenylmercury acetate release from articles in the indoor environment is not adequately controlled and may cause adverse health effects to consumers. Measurements of high levels of mercury in air (in the form of mercury vapour) in school gyms with phenylmercury catalyst in floorings clearly show that the compounds are released from articles and degraded. For the use of phenylmercury catalyst in gym floorings the majority of measurements of air concentrations of elemental mercury in school gyms reported would result in a RCR>1, which means a risk e.g. for teachers and children exposed to mercury vapour from PU floors in gymnasiums, under certain conditions. Risk was also indicated for industrial workers exposed to the phenylmercury catalysat during open application of the PU systems for casting of PU parts estimated by using ECETOC TRA tool with phenylmercury acetate (PMA).

The quantitative risk characterisation for environment indicates that the estimated concentrations of mercury (in the form of inorganic mercury resulting from emissions of the phenylmercury compounds) were below those predicted to cause an effect in the aquatic and terrestrial environment. Due to lack of data a quantitative risk assessment for secondary poisoning could not be performed.

It should also be noted that according to the estimations a large amount of mercury will accumulate in the landfills and apparently remain there. The long-term fate of mercury in the landfills is not known, evidently there is a potential for a release to the environment at a later stage.

Risk assessment of alternatives

Commonly used alternative catalysts to the five phenylmercury compounds are catalysts based on bismuth, zinc, zirconium, titanium and amines (Section C.1.2). Non-mercury catalysts seem to be available for almost all applications, total replacement require some further research and development. Based on available data, the properties of the non-mercury substances markedet as alternatives for the current use of phenylmercury catalysts are generally regarded as safer than the phenylmercury catalysts with regard to degradation in the environment, potential for bioaccumulation and toxicity (Section C.2-C.4).

Many different organic mercury compounds can be used as catalysts in polyurethane production (Section C.1.1). Other mercury catalysts than the five phenylmercury compounds have been used in the past and current manufacture, import or use in EU can not be excluded. All such organic mercury substances are classified as hazardous to health and the environment with acute and chronic effects (H330, H310, H300, STOT RE 2 H373, H400, H410), and it can be expected that these compounds will also eventually degrade to Hg in the environment. Mercury free alternatives are therefore regarded as having a lower risk.

Some organotins compounds were also mentioned as alternatives; for example for silicone and polyurethane systems, catalysts based on dibutyltin diacetate (CAS No 1067-33-0), dibutyltin dilaurate (CAS No 77-58-7), dimetylbis[(1-oxoneodecyl)oxy]stannate (CAS No 68928-76-7), dibutyltin oxide (CAS No 818-08-6) and dioctyltin dilaurate (CAS No 3648-18-8) can be used. However, entry 20 of Annex XVII of REACH already contains restrictions on organostannic compounds used as biocide in free association paint or to prevent the fouling, or used in the treatment of industrial waters. In addition, Commission Regulation (EU) No 276/2010 completes this annex XVII with a ban on tri-substituted organostannic compounds, and restrictions on dibutyltin compounds and dioctyltin compounds. These restrictions should be considered as a clear signal that organostannic compounds are not suitable alternatives.

A.2.2 Justification that action is required at community-wide basis

Action on a Community-wide basis is necessary for a global persistent pollutant like mercury (Part D). Cross boundary human health and environmental problems will not be sufficiently and effectively controlled by national actions. The life-cycle of the phenylmercury compounds leads to a significant release of mercury to the environment and adds to the overall emissions of mercury. Regulating through Community-wide action ensures justice for the producers of the substances and articles in different Member States. Based on this, mercury use and releases from the phenylmercury compounds in the EU need to be controlled on a Community-wide basis. Acting at Community level, including the proposed restriction, also strengthens the EU efforts at the global level.

A.2.3 Justification that the proposed restriction is the most appropriate Community-wide measure

Several risk management options have been assessed (see Part E for full assessment). Mainly based on the criteria of risk reduction capacity, a restriction is considered the most appropriate risk management option to reduce the use of the 5 phenylmercury compounds in question.

Two options have been considered, involving the possible restriction entering into force either five (option 1) or two years (option 2) after its assumed adoption. In terms of a comparison of the two restriction options, the risk reduction capacity of option 1 is slightly less than that of option 2 because the restriction would be implemented three years later. There would therefore be greater emissions under option 1 (those related to new uses between 2015 and 2018).

Option 2 would be less proportionate and simple to implement than option 1, because the necessary alternatives are not expected to be available for certain applications within a shorter timescale (2 years). This could lead to substantial difficulties in substituting all of the uses within this shorter timeframe, leading to greater costs and also potentially to unforeseen

consequences associated with the end uses in which the polyurethane systems are applied. Consultees indicated that substitution could be feasible within 5 years after adoption.

As numerous identified alternatives which may exhibit less risk were already applied, and as RAC considers that there are high uncertainties regarding the delay needed to put in place all alternatives (the only indication is 70% substitution within 2-3 years and no data states the improvement in term of substitutions if delay is extended from 3 to 5 years), a third option, a total ban within a 3-year delay, appears to be the most appropriate risk management measure from a risk assessment point of view.

From a socio-economic point of view no information on costs and other consequences of a 3-years phase out period (e.g. substitution by the easiest available alternatives which might be other organo-mercury compounds) is available in order to conclude on the proportionality of such an option. Consultations with industry showed that 70 % of the mercury-containing PU systems can easily be replaced within 2 – 3 years; the remaining 30 % would be more difficult and need further R&D activities. It is expected that substitution for those 30 % is possible after 3 – 5 years which leads to the conclusion that the 5 years option seems to be the most appropriate risk management measure from a socio-economic point of view. No information in order to conclude on the proportionality of the third restriction option (phase-out period of 3 years) is available.

The enforceability and manageability of option 1 is greater than that of option 2 because of the time needed for authorities and industry to adequately prepare for the restriction. Option 3 provides an intermediate situation. There is considered to be no substantial difference in the ability of those involved to monitor the effectiveness of the three options. Testing of polyurethane products in which mercury-based catalysts may be used should be based on measurements of Hg (Section E.2.1.3), cf. limit value specified in A.1.2 and other EU-legislation on some of the same mercury compounds (Cosmetics Regulation EC/1223/2009). If deemed necessary to test for the organomercury compounds included in the proposed restriction, analytical methods including sampling and preparation methods must be further developed.

Although option 2 – a restriction introduced over two year period – is likely to lead to a greater overall reduction in releases of mercury to the environment than option 1, it is the conclusion of the dossier submitters assessment that option 1 would be the preferred option of the two. This is because there is evidence from the industry using the substances that there would be technical difficulties in replacing the substances over a period shorter than five years, although probably not for all uses. In order to avoid the potential unforeseen consequences of a restriction over a shorter period, it would seem prudent to allow sufficient time for the replacement of these substances to take place. There is insufficient information available to determine how a stepwise phase-out of the substances could be achieved so the impacts of such an approach have not been investigated in depth.

RAC has refined the calculations and proposes a new option with a 3 years delay for entering into force. SEAC considered that from a socio-economic point of view the dossier submitters' proposal for option 1 seems appropriate.

A.2.4 Socio-economic analysis

Due to limited information, especially on the issue of imported articles, it has only been possible to perform a partial SEA.

On the basis of the available information it seems clear that a restriction on the 5 phenylmercury compounds will give significant reductions in mercury emissions. As described above the health and environmental benefits of reducing mercury emissions are significant. It has not been possible to quantify and monetize the exact benefits of reduced emissions of the 5 phenylmercury compounds subject to the restriction. However, a survey of different studies performed in the restriction dossier for mercury in measuring devices (ECHA 2010, Appendix 2) indicates a benefit estimate between € 5 000 – 20 000 per kg Hg reduced. These estimates have been considered further in order to decide on the proportionality of the restriction proposal, especially as far as the inclusion of manufacture in the scope of the restriction is concerned.

It is expected that all use of mercury-containing catalysts can be replaced within a transition period of 5 years. A shorter transition period will lead to increased costs due to reduced quality of products. Alternatively derogations might be given leading to increased administrative costs. The main cost of restricting the use of these substances will be the cost of finding and developing suitable alternatives. The cost-effectiveness of the proposed restriction is estimated to be 649 €/kg (see Part F).

There are no benefit estimates which are fully transferable to the emission reductions estimated. However, the lowest estimate of the benefits presented above, outweighs the estimated costs of the restriction by a large margin as far as a restriction on placing on the market and use is concerned. The cost-benefit ratio of restricting manufacture is mainly dependent on two factors, i.e. the behaviour of actors outside the EU (substitution of phenylmercury-containing catalysts by mercury-free catalysts) as well as the amount of mercury emissions (from exports) likely to come back to the EU (due to the long-range transport –LRT- properties of the substances). These factors are highly uncertain but calculations show that the costs are not disproportionate to the benefits (see part F). Bearing all the uncertainties in mind we believe that this merit the conclusion that the benefits of the restriction proposed can be expected to outweigh the costs.

Many other organomercury compounds can be used as catalysts in polyurethane production. The actual use within the EU is most probably limited to a small number, see Section C.1.1.7. The 5 substances that have been included in this restriction proposal are those that are or have been used and manufactured in EU in significant amounts. Use of other organomercury catalysts, now or in the future, cannot be excluded. However, restricting the use of all mercury compounds as catalysts would most probably not incur any additional costs of significance.

As mentioned above, no information is available on the use of any mercury compounds in imported articles.

B INFORMATION ON HAZARD AND RISK

Introductory remarks

The assessment of the five phenylmercury compounds per se is mainly based on data for phenylmercury acetate since the majority of available published papers are studies on this substance. The risk related data is presented in Section B.1 to B.10. Due to the fact that the phenylmercury compounds are degraded to hazardous degradation products, i.e. two-valent mercury and elemental mercury, which under certain environmental conditions are transformed into methylmercury, information about effects and potential risks from the degradation/transformation products has been included as well. A complete discussion on the risks of mercury and mercury compounds is beyond the scope of this restriction proposal. Several approved international reviewed reports were used in this proposal to assess the risk from elemental mercury, inorganic mercury and methylmercury. These documents were developed to document the need for action against mercury pollution. Information on hazard, emission and risk was found in the report "Global mercury assessment" (UNEP, 2002) developed to form a better basis for considering the need for international action on mercury and its compounds, and in the follow-up report on emission estimates (UNEP Chemicals Branch, 2008). Among the central documents were also "Guidance for Identifying Populations at Risk from Mercury Exposure" (UNEP, 2008), which was intended to inform countries concerned about the potential health impacts of mercury pollution and, if necessary, to assist in identifying specific subpopulations that may be at risk. Relevant reports of meetings and monographs prepared by the Joint FAO/WHO Expert Committee on Food Additives (JECFA) were taken into account in the development of this guidance document as part of international recommendations on mercury and methylmercury in fish and other food (FAO/WHO, 2007; FAO/WHO, 2003; WHO, 2000). For the assessment of risk to human health from elemental mercury, inorganic mercury and methylmercury the peer reviewed reports from WHO (2003) and ATSDR (1999) were central, as well as the peer reviewed mercury study report from EPA (1997). In addition documents from SCHER (2008) and SCENIHR (2008) concerning environmental risks and indirect health effects from mercury in dental amalgam were used as references. These committees were established by the European Commission to provide them with scientific advice relating to consumer safety, public health and the environment.

To facilitate the reading, a short summary of mercury in the environment, the environmental forms of mercury, exposure and target organs is provided below (UNEP, 2002; UNEP 2010a, b).

Mercury is found both naturally and as an introduced contaminant in the environment. Anthropogenic emissions have widespread impacts on human and environmental health. Mercury is considered to be a global persistent pollutant; in the environment it cannot be broken down to any harmless form. Once emitted, mercury enters the complex biogeochemical cycle. After intensive use of mercury over many years mercury can be found in almost all environmental compartments, like the atmosphere, soil and water systems and in biota all over the world. The formation of methylmercury and subsequent biomagnification in food chains are of serious concern.

Mercury exists in the environment in several forms: elemental (metallic or Hg0), inorganic (monovalent and divalent Hg and their complexes), and organic mercury (e.g., methylmercury, thiomerosol). The form of the mercury affects its absorption, toxicokinetics,

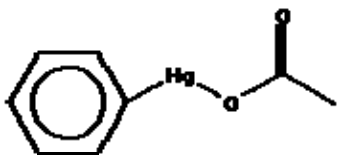
retention and ultimately the body burden. Methylmercury is the most toxic form of mercury found in the environment. Exposure to methylmercury occurs from intake of fish, shellfish and marine mammals.
The primary targets for toxicity of mercury and mercury compounds are the nervous system, kidneys, and the cardiovascular system. Other organ systems that may be affected include the respiratory, gastrointestinal, hematologic, immune, and reproductive systems. It is generally accepted that the developing nervous system is the most sensitive target organ to the toxic effects of mercury.
Based on a comparison of the properties of methylmercury with the REACH PBT-criteria it is concluded that methylmercury is a PBT-like substance (or substance of equivalent concern). According to REACH, if transformation/degradation products with PBT-properties are being generated, the substances themselves must be treated like PBT-substances with regard to emission estimation and exposure control. To this end, the exposures and emissions to humans and the environment should be minimized to the extent possible, and the main objective of the emission characterisation is to estimate the amounts of the substance released to the different environmental compartments.

Due to lack of data, but also due to the fate of phenylmercury compounds in the environment it is proposed to also perform a quantitative risk assessment for environment on the basis of the inorganic mercury data. Only a very approximate quantitative risk characterisation could be performed. It should be borne in mind that a piece by piece risk assessment of releases of mercury and mercury compounds from single product groups does not give the full picture of the risks, for that purpose different sources of releases would have to be combined. This is outside the scope of this report.

RAC considers that if transformation/degradation products with PBT-properties are being generated, the substances themselves must be treated like PBT-substances with regard to emission estimation and exposure control. For this reason, discussions of risks based on PEC/PNEC considerations in the background document are not of particular relevance to the opinion. The assessment presented by Norway as dossier submitter is reproduced below for transparency.

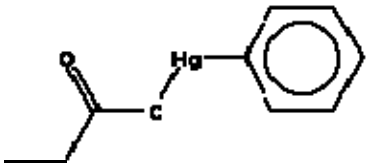
B.1 Identity of the substances and physical and chemical properties

B.1.1 Phenylmercury acetate

EINECS name	Phenylmercury acetate
IUPAC name:	Phenylmercury acetate
EC number:	200-532-5
Cas number:	62-38-4
Index number:	080-011-00-5
Synonyms	Mercury, (acetato)phenyl- ; Mercury, (acetato-O)phenyl-; Phenylmercury acetate; (Acetato-O)phenylmercury; Acetatophenylmercury; Acetic acid, phenylmercury deriv.; Acetoxyphenylmercury; Agrosan; Agrosan D; Algimycin 200; Anticon; Antimucin WBR; Antimucin WDR; Benzene, (acetoxymercurio)-; Bufen; Bufen 30; Ceresol; Contra Creme; Femma; Fungicide R; Fungitox OR; Hexasan; Hexasan (fungicide); Intercide 60; Intercide PMA 18; Liquiphene; Lorophyn; Meracen; Mercron; Mercuriphenyl acetate; Mercuron; Mergal A 25; Mersolite 8; Mersolite D; NSC 35670; NSC 61321; Neantina; Norforms; Nuodex PMA 18; Nylmerate; PMA; PMA (fungicide); PMA 220; PMAC; PMAS; Panomatic; Parasan; Parasan (bactericide); Phenylmercuric acetate; Phix; Programin; Quicksan; Ruberon; Samtol; Sanitized SPG; Sanmicron; Scutl; Seed Dressing R; Seedtox; Setrete; Spruce Seal; Tag; Tag 331; Tag Fungicide; Tag HL 331; Trigosan; Troysan 30; Troysan PMA 30; Verdasan; Volpar; Zaprawa Nasienna R; Ziarnik
Molecular Formula	$C_8H_8HgO_2$
Structural Formula	
Molecular weight (g/mole)	336.75

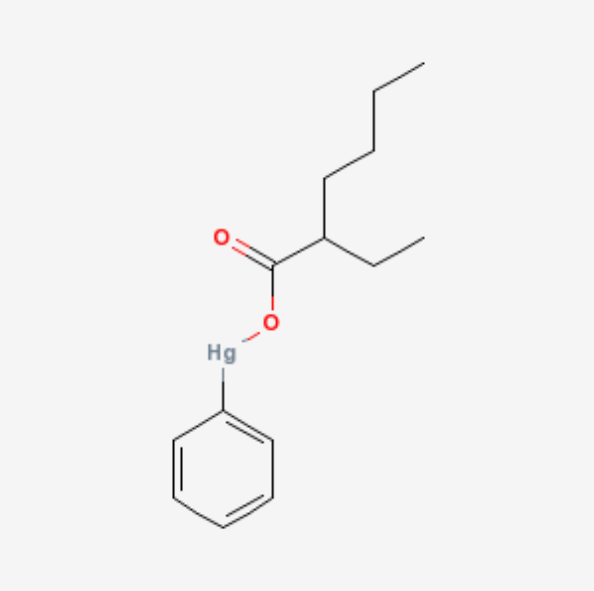
Property	Value
Physical state at 20°C and 101.3 kPa	Odourless, hygroscopic white or white-yellow crystalline powder (InChem, 2009)
Melting/(freezing) point	149-153 ºC (eChemPortal, 2009)
Boiling point	No data found
Relative density	No data found
Vapour pressure	$6.00x10^{-6}$ mm Hg (at 20 °C) (ChemID, 2009) 1.2 mPa (35 ºC) (Tomlin, 1997) 0.016 Pa (at 25 °C) (International chemical safety cards, WHO/IPCS/ILO)
Surface tension	No data found
Water solubility	4370 mg/L (15 °C) (ChemID, 2009) 1843 mg/L estimated with QSAR Episuite (see Appendix 2)
Partition coefficient n-octanol/water (log value)	0.71 (ChemID, 2009) 0.89 estimated with QSAR Episuite (see Appendix 2)
Flash point	37.8 °C (IPCS INCHEM)
Flammability	No data found
Explosive properties	No data found
Self-ignition temperature	No data found
Oxidising properties	No data found
Granulometry	No data found
Stability in organic solvents and identity of relevant degradation products	No data found
Dissociation constant	$1,5x10^{-5}$ (Parikh SS, Sweet TR; 1961)
Viscosity	No data found
Auto flammability	No data found
Reactivity towards container material	No data found
Thermal stability	No data found
Decomposition Temperature (°C)	No data found
Vapour Density (air=1)	11.6 (InChem, 2009)
Henry's Law constant (atm/m^3/mol at °C)	$5.66x10^{-10}$ atm*m^3/mole (at 25 °C) (ChemID, 2009)
pK_a	No data found
Migration potential in polymer	No data found

B.1.2 Phenylmercury propionate

EINECS name	Phenylmercury propionate
IUPAC name	Phenylmercury propionate
EC number	203-094-3
Cas number	103-27-5
Synonyms	Mercury, phenyl(propanoato-κO)- Mercury, phenyl(propanoato-O)-; Mercury, phenyl(propionato)-; Mercury, phenyl(propionyloxy)-; Phenylmercury propionate; Metasol 57; Metasol P-6; NSC 11822; Phenyl(propionyloxy)mercury; Phenylmercuric propionate
Molecular Formula	$C_9H_{10}HgO_2$
Structural Formula	
Molecular weight (g/mole)	350.76

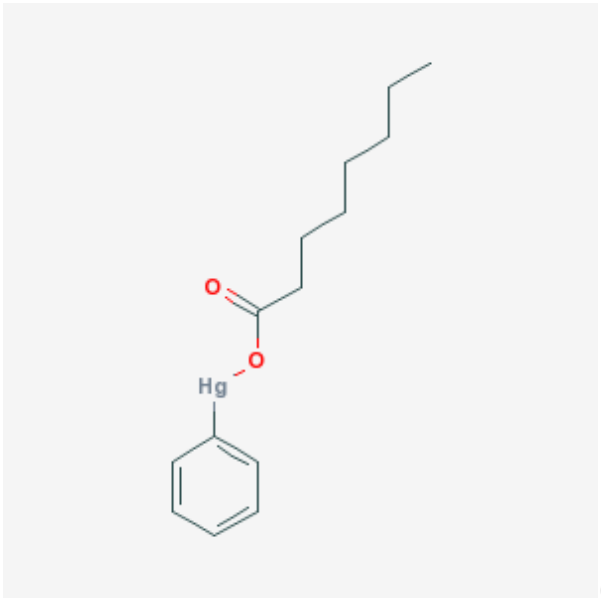
Property	***Value***
Physical state at 20°C and 101.3 kPa	White to off-white wax-like substance /14 + 15/
Melting/freezing point	65-70ºC (Sigma-Aldrich, 2009)
Boiling point	No data found
Relative density	No data found
Vapour pressure	No data found
Surface tension	No data found
Water solubility	405.6 mg/L estimated with QSAR Episuite (see Appendix 2)
Partition coefficient n-octanol/water (log value)	1.38 estimated with QSAR Episuite (see Appendix 2)
Flash point	No data found
Flammability	No data found
Explosive properties	No data found
Self-ignition temperature	No data found
Oxidising properties	No data found
Granulometry	No data found
Stability in organic solvents and identity of relevant degradation products	No data found
Dissociation constant	$3.1x10^{-5}$ (Parikh SS, Sweet TR; 1961) $1.5x10^{-5}$ (Tang and Nielsen, 2010; appendix 12)
Viscosity	No data found
Auto flammability	No data found
Reactivity towards container material	No data found
Thermal stability	No data found
Decomposition Temperature (°C)	No data found
Vapour Density (air=1)	No data found
Henry's Law constant (atm/m^3/mol at °C)	No data found
pK_a	No data found
Migration potential in polymer	No data found

B.1.3 Phenylmercury 2-ethylhexanoate

EINECS name	(2-ethylhexanoato) phenylmercury (ESIS, 2009)
IUPAC name	Phenylmercury 2-ethylhexanoate
EC number	236-326-7
CAS number	13302-00-6
Synonyms	Mercury, (2-ethylhexanoato-κO)phenyl- Mercury, (2-ethylhexanoato)phenyl-; Mercury, (2-ethylhexanoato-O)phenyl-; Mercury, [(2-ethylhexanoyl)oxy]phenyl-
Molecular Formula	$C_{14}H_{20}HgO_2$
Structural Formula	
Molecular weight (g/mole)	420.89

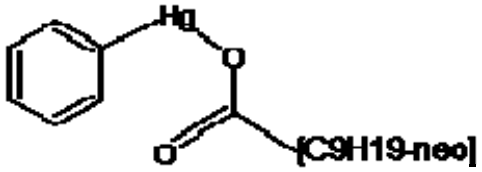
Property	***Value***
Physical state at 20°C and 101.3 kPa	No data found
Melting/freezing point	No data found
Boiling point	No data found
Relative density	No data found
Vapour pressure	No data found
Surface tension	No data found
Water solubility	1.4 mg/L estimated with QSAR Episuite (see Appendix 2)
Partition coefficient n-octanol/water (log value)	3.76 estimated with QSAR Episuite (see Appendix 2)
Flash point	No data found
Flammability	No data found
Explosive properties	No data found
Self-ignition temperature	No data found
Oxidising properties	No data found
Granulometry	No data found
Stability in organic solvents and identity of relevant degradation products	No data found
Dissociation constant	No data found
Viscosity	No data found
Auto flammability	No data found
Reactivity towards container material	No data found
Thermal stability	No data found
Decomposition Temperature (°C)	No data found
Vapour Density (air=1)	No data found
Henry's Law constant (atm/m^3/mol at °C)	No data found
pK_a	No data found

B.1.4 Phenylmercury octanoate

EINECS name	Not listed in EINECS
IUPAC name	Phenylmercury octanoate
EC number	
CAS number	13864-38-5
Synonyms	Mercury, (octanoato)phenyl-; NSC 122854; Phenylmercuric octanoate
Molecular Formula	$C_{14}H_{20}HgO_2$
Structural Formula	 (
Molecular weight (g/mole)	420.89

Property	***Value***
Physical state at 20°C and 101.3 kPa	No data found
Melting/freezing point	77-80^{o}C Geraci, John; Chodsky, Sergey V.; Phenylmercury salts of branched chain aliphatic monocarboxylic acids Patent No: US 3304316
Boiling point	No data found
Relative density	No data found
Vapour pressure	No data found
Surface tension	No data found
Water solubility	1.2 mg/L estimated with QSAR Episuite (see Appendix 2)
Partition coefficient n-octanol/water (log value)	3.84 estimated with QSAR Episuite (see Appendix 2)
Flash point	No data found
Flammability	No data found
Explosive properties	No data found
Self-ignition temperature	No data found
Oxidising properties	No data found
Granulometry	No data found
Stability in organic solvents and identity of relevant degradation products	No data found
Dissociation constant	$2.4x10^{-5}$ (Tang and Nielsen, 2010; appendix 12)
Viscosity	No data found
Auto flammability	No data found
Reactivity towards container material	No data found
Thermal stability	No data found
Decomposition Temperature (°C)	No data found
Vapour Density (air=1)	No data found
Henry's Law constant (atm/m^3/mol at °C)	No data found
pK_a	No data found

B.1.5 Phenylmercury neodecanoate

EINECS Name	(neodecanoato-O)phenylmercury (ESIS, 2009)
IUPAC name	Phenylmercury neodecanoate
CAS number	26545-49-3
EC number	247-783-7
Synonyms	Mercury, (neodecanoato-κO)phenyl- Mercury, (neodecanoato)phenyl-; Mercury, (neodecanoato-O)phenyl-; Neodecanoic acid, mercury complex
Molecular Formula	$C_{16}H_{24}HgO_2$
Structural Formula	
Molecular weight (g/mole)	448.955

Property	***Value***
Physical state at 20°C and 101.3 kPa	Liquid (STN Easy, 2009)
Melting/freezing point	No data found
Boiling point	No data found
Relative density	No data found
Vapour pressure	No data found
Surface tension	No data found
Water solubility	0.14 mg/L estimated with QSAR Episuite (see Appendix 2)
Partition coefficient n-octanol/water (log value)	4.71 estimated with QSAR Episuite (see Appendix 2)
Flash point	No data found
Flammability	No data found
Explosive properties	No data found
Self-ignition temperature	No data found
Oxidising properties	No data found
Granulometry	No data found
Stability in organic solvents and identity of relevant degradation products	No data found
Dissociation constant	8.2×10^{-5} (Tang and Nielsen, 2010; appendix 12)
Viscosity	No data found
Auto flammability	No data found
Reactivity towards container material	No data found
Thermal stability	No data found
Decomposition Temperature (°C)	No data found
Vapour Density (air=1)	No data found
Henry's Law constant (atm/m^3/mol at °C)	No data found
pK_a	No data found
Migration potential in polymer	No data found

B.1.6 Justification for grouping

The assessment covers the five phenylmercury compounds phenylmercury acetate, -propionate, -octanoate, -2-ethylhexanoate and -neodecanoate. The identified use in the EU + EFTA of the five phenylmercury compounds today is the use as a catalyst in the production of polyurethane. Most information is available for phenylmercury acetate, however, quantum chemical calculations (Tang and Nielsen, 2010; see appendix 12) showed that the five phenylmercury compounds have a similar fate and hazard profile. These calculations revealed that once the phenylmercury carboxylates are released into the environment and come in contact with water, all five compounds are immediately transformed to a common intermediate (phenylmercury hydroxide) that can be further degraded to inorganic mercury. Furthermore, atmospheric lifetimes of all phenylmercury carboxylates are expected to be very similar. All five phenylmercury compounds are degraded to inorganic mercury and elemental mercury, which can be transformed to methylmercury. Due to structural similarity, grouping of the five compounds seems justified. Further, the similar chemical properties of the five phenylmercury compounds trigger for their similar technical function as catalyst in the polyurethane production, as evidenced by their historic, current or potential use for this purpose. To avoid easy substitution by each other the group of phenylmercury acetate, -propionate, -octanoate, -2-ethylhexanoate and -neodecanoate is proposed to be restricted.

RAC considers that regarding the chemical breakdown similarities, it is fully justified to group the 5 phenylmercury compounds. The cycling of mercury in the biosphere entails that the source of this transformation product is always present once released. Furthermore, as other phenylmercury compounds are expected to follow the same degradation pathway as the 5 phenylmercury compounds in nature and thereby represent an equivalent risk; RAC recommends that it is made clear that any other mercury compound is not suitable as alternative.

B.2 Manufacture and uses

Based on information in the report "Options for reducing mercury use in products and applications and the fate of mercury already circulating in society" (Cowi and Concorde East/West, 2008) the uses of certain phenylmercury compounds as catalysts in polyurethane systems were identified as significant applications of mercury. It was stated that the phenylmercury compounds are manufactured and used in extensive amounts in Europe and that no other mercury chemicals are used in such large volumes in Europe. The restriction proposal focuses on phenylmercury compounds mainly used as catalysts in the production of polyurethane (PU).

Phenylmercury compounds have been used for several purposes. 71 phenylmercury compounds are included in EINECS. 33 phenylmercury compounds or mixtures thereof were pre-registered to ECHA in 2008, see Appendix 9. None of the pre-registered phenylmercury compounds were registered by 30 November 2010.

In Part C the possibility of using other mercury compounds as catalysts in the production of polyurethane is discussed, in addition to alternative non-mercury catalysts.

B.2.1 Manufacture and import of a substance

Production
Less than four manufacturers of the five phenylmercury compounds in the EU+EFTA have been identified. The total reported production volumes in 2008 were as follows:

- Phenylmercury neodecanoate: 75-150 tonnes
- Phenylmercury acetate: 5-10 tonnes
- Phenylmercury 2-ethylhexanoate: 50-100 tonnes
- Phenylmercury octanoate: no production identified
- Phenylmercury propionate: no production identified

The actual quantity manufactured is known, but cannot be provided for confidentiality reasons. The actual quantity is not identical with the mean value, but is a value within the indicated range.

The majority of phenylmercury 2-ethylhexanoate and phenylmercury acetate is exported to countries outside EU whereas a significant part of the phenylmercury neodecanoate is used within the EU+EFTA.

According to the major manufacturer of three of the substances, the substances are produced as pure substances with >99% purity. No data are available from the manufacturer on any impurities.

The substances are formulated into catalysts by the manufacturers manufacturing the substances. The reported releases from manufacture thus represent the releases from manufacture of the substance and the formulation of the catalyst. It would not be possible to allocate the releases to each of the two processes. Neither is it possible to allocate the releases to the individual substances, but they may roughly be allocated on a tonnes/tonnes basis.

The concentration of the substances in the catalyst product (mixture) is as follows, the rest is taken up by solvents:

Phenylmercury neodecanoate: 80%
Phenylmercury 2-ethylhexanoate: 42%
Phenylmercury acetate: 30%.

The solvents used by one of the manufacturers in the EU have been informed to be “solvent naphtha (petroleum), light arom.” (CAS No. 64742-95-6). For a similar catalyst based on phenylmercury neodecanoate, produced outside the EU, it is reported that the solvent is neodecanoic acid (Vertellus 2009a).

Import

Mercury compounds are covered by the Rotterdam Convention therefore import and export of the substances from/to the EU shall be notified by the importing/exporting company to the Designated National Authority (DNA) in each country. In the EU the DNA compiles and aggregates the information received and transmits it to the Commission, who publish an overall non-confidential summary on the Internet. According to the European Database Export Import of Dangerous Chemicals (EDEXIM) only one notification of import of the substances into the EU was recorded in EDEXIM in 2008: import of phenylmercury acetate from Switzerland.

A major European supplier of chemicals for the laboratory sector informed that they in 2007 imported phenylmercury acetate from a supplier in the U.S.A (amount not indicated), but that phenylmercury acetate will no longer be on the product list of the company. This import is not recorded in EDEXIM.

Import of mercury containing catalysts for PU production is not reported in EDEXIM. A catalyst (containing phenylmercury neodecanoate) for PU production produced in the U.S.A. is marketed in the EU, but no data on the amounts imported have been provided by the importer. Based on market considerations it is estimated that the imported quantity in 2008 was most likely less than 5 tonnes.

Export

According to EDEXIM, Germany and Spain accounted for the entire export of mercury compounds from the EU in 2008 and the same was true for the previous years. In 2008 the number of export notifications for mercury compounds was 62. In the published summary on EDEXIM the mercury compounds are only indicated as "mercury compounds" and it is not clear how many of the notifications concern phenylmercury compounds. For 2009 (until Nov 2009) 8 export notifications for “phenyl mercuric neodecanoate_80%” are registered.

According to information provided by the European Commission, 15 tonnes phenylmercury acetate was exported from Germany in 2006. No newer information has been available.

The export of catalyst (containing phenylmercury neodecanoate) from Spain to a number of countries is specifically indicated under "preparations" with 9 registered export notifications from Spain in 2008. According to COWI and Concorde East/West (2008) 40 tonnes of PU catalyst (corresponding to approximately 30 tonnes phenylmercury neodecanoate) were

exported to countries outside the EU in 2006, but the exported quantities probably vary considerably from year to year.

Summary

Table B-1summarises the available information on production, export and import of the substances as pure chemicals or in preparations. The import and export has been estimated on the basis of knowledge on produced volumes and the estimates on the quantities used in the EU+EFTA as described in the next section.

Besides, the substances may be imported and exported in articles, first of all in parts made of polyurethane elastomers. No attempts have been done in estimating the import and export in articles, but imported products may account for a significant part of the end-uses of the substances. Europe represents some 20-30% of the global use of mercury catalysts for production of products (COWI and Concorde East/West, 2008) and in the absence of specific data on import and export with articles, it is for the estimates on the releases from the use phase and waste disposal assumed that the total mercury import in articles balance the export. However, as phenylmercury 2-ethylhexanoate seems to be used in more significant amounts outside the EU (as indicated by the significant export of the substance), imported products may account for a major part of this compound in used articles if the phenylmercury 2-ethylhexanoate is used as catalyst in polyurethane production.

Table B-1 Estimated production, export and import of the substances as pure chemicals or in preparations in 2008 in tonnes (import/export in articles not included)

CAS number	62-38-4		103-27-5		13302-00-6		13864-38-5		26545-49-3			
2008	Phenylmerury-											
(as pure chemical: in articles not included)	acetate		propionate		2-ethylhexanoate		octanoate		neodecanoate		Total PhHg	
Produced	5	10	0	0	50	100	0	0	75	150	**130**	**260**
Export	5	10	0	0	49	99	0	0	39	85	**93**	**194**
Import	1	0	0	0	0	0	0	0	0	5	**1**	**5**
Use in EU+EFTA	1	0	0	0	1	1	0	0	36	70	**38**	**71**
										exported/used	2.4	2.7
											Total Hg	
	acetate		2-ethylhexanoate		neodecanoate					**Produced**	**60**	**121**
Hg/PhHg ratio	0,5957		0,4766		0,4468					**Export**	**44**	**91**
										Import	**1**	**2**
										Use in EU+EFTA	**17**	**32**
										exported/used	2.6	2.9

Note: considering the phenylmercury compounds quantities, the ratio “quantity exported / quantity used in EU” can be estimated between 2.4 and 2.7. The mercury/phenylmercury compound mass ratios are different among the 3 used phenylmercury compounds. When converting the quantities in mercury equivalent, the ratio “quantity exported / quantity used in EU” can be estimated between 2.6 and 2.9.

B.2.2 Uses

In the polyurethane manufacture, the catalysts are used for catalysing the reaction between a polyol and an isocyanate component, i.e. for hardening or curing the polyurethane. A two-component PU system consists of a polyol component and an isocyanate component which is mixed by the application of the system. The catalyst is typically included in the polyol component.

For many applications, the catalysts of choice for catalysing the reaction between the polyol and an isocyanate composition, i.e., for hardening or curing polyurethane (PU) materials, have long been organic mercury compounds. This is because, for a wide range of polyurethane materials, these catalysts provide a robust and desirable "reaction profile" characterised by:

- an initial induction period in which the reaction is either very slow or does not take place,which continues for sufficient time to permit the "system" (combination of polyurethane materials and catalyst) to be mixed and cast (or sprayed); and
- a subsequent rapid reaction period during which the product cures, taking on its final properties (shape, hardness, flexibility, strength, etc.).

There are special properties sometimes required of these catalysts, like long "pot life", with a sharp viscosity rise toward the end of the reaction, followed by a "fast" curing of the part. In contrast to PU foam manufacture, the formation of bubbles and foam is undesirable in polyurethane elastomer production. For this reason, heavy metals such as mercury have long been used in catalysts as they exhibit the high reactivity and selectivity required in the process.

A reasonable induction time (also known as the "gel time" or "pot life") before hardening, which may be easily varied when using a mercury catalyst, e.g. by changing the amount of catalyst added, is desirable because it allows the liquid reaction mixture to be cast (poured or moulded) after addition of the catalyst, and therefore gives the user more control over the application. A rapid and complete reaction after the gel time is important to provide finished articles that are not sticky and that develop their desired physical properties quickly after casting, which allows fast turnaround in the production facility or at the site of application (COWI and Concorde East/West, 2008).

Applications of the PU system with mercury catalyst

By the application (processing) of the PU system the two components are mixed together and poured into a mould or applied by other means. Different processes are applied and the following gives some examples provided by formulators[3] of the PU systems. The examples concern small-scale application of the PU system.

According to industry contacts, in large-scale production automated moulding systems, where the curing can be controlled by heating, is applied. The better control of the curing process in these systems means that in general it has been easier to replace the mercury catalysts by alternatives.

-Systems for repair work

According to one formulator of PU systems that are used for repairing expansion joints, rebuilding and resurfacing PU elastomer parts the two components are mixed together in small amounts (<2 kg typically). The mercury catalyst is contained in only one of these component parts at <1.5%. The product is applied by hand via a brush or tool.

- Systems for hand casting

[3] The information concerning different applications (processing) has been provided by formulors of the two component systems.

The following (shortened) instruction for a hand-casting PU systems for prototyping, embedding or any type of clear casting gives an example of the application of the systems (Kemitura, 2010):

Mould Preparation:	Ensure that the mould is clean and dry.
Resin Preparation:	Check the Part B (isocyanate) for any signs of crystallisation. If there are any crystals, warm the container (with the lid firmly on) to 45-60 ºC until the crystals disappear. Always cool the Part B to room temperature before using. When pigmenting, ensure that the pigment is not water based, and never use more than 5% in the Part A.
Mixing instructions:	Mix the two components in the correct ratio, mixing carefully to avoid air inclusion. The material will be cloudy in appearance for 2-3 minutes. Continue mixing until the liquid becomes clear. Degas for approx. 3 minutes before pouring. Pour the material into the mould, onto the sides in order to reduce air bubbles. Degas if necessary, avoid boiling the material at very high vacuums.
Curing:	The casting can generally be demoulded in 1-2 hours at room temperature. If the casting has thin sections, it is advisable either to use preheated moulds (40-50ºC), or to postcure the castings after gelation in an oven at 40-50ºC. Leave the casting for at least 48 hours before machining or polishing; ensure that the material does not reach temperatures above 60ºC during machining or polishing, or it may distort.
Polishing tips:	For general polishing of a moulded part use a fine liquid polish. If a deep scratch needs to be removed then wet and dry paper should be used in the following descending grit sizes 400, 800, 1000 and 1200.

The described process involves polishing of the moulded part. Industry contacts have indicated that polishing is not common for elastomer parts.

- Systems for encapsulations

The following description relates to the use of the PU systems for encapsulation: In electronics and electrical systems (e.g. light emitting components), joints and cable connector encapsulation protect assemblies from ingress of fluids; in acoustic and sonar applications encapsulation of components and assemblies gives strength to the assembly and protect it from the environment in which it is operating.

The mercury catalysed PU parts are almost all hand mixed. The maximum size of hand mix that is carried out is 2 – 3 kg. The other end of the scale is a 100 g mix. The total mercury content will be 0.05% to 0.1% (as phenylmercury neodecanoate). The polyol and isocyanate components are weighed out in the correct ratio to produce the part required.

The polyol and isocyanate components are then mixed for a specified time. The reacting mix is transferred to a vacuum chamber where all mixed-in air is removed. The mix is then introduced into the mould using a number of methods. The casting usually takes place in several steps where electronic components are inserted into the mould between each cast gradually building up the encapsulated electronics.

All of the mercury catalysed materials are bulk cast. The curing generates heat internally which accelerates the PU reaction. The amount of catalyst required in the PU system will

depend on a number of factors such as geometry of the part, moulding time required by the customer, and heat sensitivity of any embedded electronic components. The heat generation is depending on the size of the mould and in larger moulds in general the concentration of catalyst is smaller. Examples of these effects in the extreme according to information from an industry contact:

- A thin wall casting of a prototype mobile phone display window needed to be cast at 80°C with a high level of catalyst (1.5%). This was because the thickness of the window was about 0.2 mm, and the part had to be fully cured and rigid when demoulded.
- A large clear resin sculpture required over 1 tonne of material to be cast in a metre cube. The catalyst level was about 0.001% and the cure was over 3 days. Any faster reaction than this resulted in too much heat being generated and the sculpture distorting and cracking.

The PU systems are not applied as coatings so the surface area to volume ratio is low. Typically the surface area of the mould would be in the range of 100 to 500 cm2 and the cast is build up in several layers.

The formulator notes that there will be some transport of catalyst near the surface of the casting to the environment, but no data to quantify this has been available.

Phenylmercury neodecanoate

The major use of the five phenylmercury compounds in the EU and EFTA countries today is the use of phenylmercury neodecanoate as a catalyst in production of polyurethane (PU) coatings, adhesives, sealants and elastomers (often referred to as CASE applications). The catalyst product is formulated by mixing of the phenylmercury neodecanoate with other compounds e.g. neodecanoic acid. The formulation of the catalyst product takes place by less than four companies in the EU.

The specific properties of the phenylmercury neodecanoate catalyst are further described in Section C.1 in the context of the discussion of alternative solutions.

Two catalyst products with phenylmercury neodecanoate have been identified, but more may be marketed: Thorcat 535 and Cocure® 55. One of the products is produced within the EU. Thorcat 535 contains 35% mercury (COWI and Concorde East/West, 2008) (=78% phenylmercury neodecanoate by weight) while Cocure® 55 contains 60-70% (by weight) phenylmercuric neodecanoate (Vertellus 2009a).

The Cocure® 55 is a mixture of phenylmercury neodecanoate and neodecanoic acid (Vertellus 2009a). The mixture is a clear, yellow, viscous liquid with a mild odour. The boiling point is 200ºC and the vapour pressure <5 mm Hg at 20ºC.

Like any catalyst used in PU systems, the mercury catalyst is incorporated into the polymer structure and remains in the final product, e.g. in elastomer coatings for leather finishing, textile and fibre treatment or coating of computer parts. The catalyst is added to the polyurethanes at levels of 0.2-1%, depending on the other components, the desired properties of the polymer, etc. Consequently the phenylmercury neodecanoate concentration in the polyurethane material is in the order of 0.1-0.6%.

It is estimated that 300-350 tonnes/year of mercury catalyst may be used globally in PU elastomer applications, of which some 60-105 tonnes/year in the EU (COWI and Concorde East/West, 2008). The report use the term ”elastomer”, which is the main application area, but the estimate seems to cover all CASE applications. This corresponds to an EU + EFTA consumption of approximately 36-70 tonnes phenylmercury neodecanoate. With 44.7% mercury it corresponds to a total mercury content of approximately 16-31.3 tonnes/year. The estimate has for this report been confirmed by the major supplier of the catalysts as being reasonable. Further < 1 tonnes of other phenylmercury compounds (phenylmercury acetate and phenylmercury 2-ethylhexanoate) may be used for the production of PU systems.

For the estimation of the releases to the environment maximum figures for the use of phenylmercury neodecanoate in EU + EFTA will be applied for worst case estimates: 70 tonnes phenylmercury neodecanoate per year corresponding to 31.3 tonnes Hg per year.

According to a major manufacturer of PU catalysts, the mercury consumption was probably 2-3 times higher 10 years ago, but no actual data have been available for the late 1990´ies. None of the substances were reported by EU Industry as an HPVC or LPVC according to Council Regulation (EEC) No 793/93 on the evaluation and control of the risks of existing substances. HPVCs (High Production Volume Chemicals) were those substances which had been imported or produced in quantities exceeding 1000 tonnes per year and produced/imported between March 23, 1990 and March 23, 1994. LPVCs (Low Production Volume Chemicals) were those substances which had been imported or produced in quantities between 10 and 1000 tonnes per year during the same reference period.

The mercury-catalyzed PU two-component systems with phenylmercury neodecanoate are in particular used for the following CASE applications:

- Spraying onto a surface as insulation or corrosion protection (coating);
- Adhesives.
- Sealants and filling materials;
- Casting of complex shapes of PU elastomers (poured or injected into a mould); Elastomers are polymers with the property of elasticity and are sometimes designated “synthetic rubbers”.

According to a major supplier of catalysts, elastomers take up about 90% of the market of mercury catalysts while about 10% is used for sealants. For adhesives and coatings, according to the supplier, the mercury use is today small while organotin or amine catalysts are the major catalysts for these applications. However, other information indicates that the mercury catalysts are still widely used for coatings.

The applications can be exemplified with the recommended application of the catalysts for PU systems: Cocure 55® is recommended for polyurethane elastomer and polyurethane coating applications in automotive, electronic, sealant, and shoe sole end-use markets (Vertellus 2009a).

Table B-2 illustrates the wide range of applications of some of the PU systems for which Material Safety Data Sheets, specifically indicating the presence of phenylmercury neodecanoate, have been available.

Table B-2 Examples of applications of PU systems with mercury catalyst specifically mentioned by suppliers

Application	Product
Two-component, elastomeric materials for repairing, rebuilding or creating rubber. Applications include pumps, diaphragms, drive couplings, flexible moulds, shock absorbers, guide bearings, rubber linings, seals, deburring machines, ship fenders, filter casings and conveyor belts.	The Belzona 2100 series (UK) (Belzona, 2009)
2-component polyurethanes that cure at room temperature to tough rubber-like materials, remaining flexible at temperatures down to even -60°C. For making**:** Vibration dampers, assembling jigs, flexible seals, rubber-like prototypes, foundry patterns and forms For repairs on**:** Conveyor belts, solid rubber tyres, conveyor rollers For coatings on: Rollers, centrifuges, polishing drums, tanks, chutes and funnels, pumps, bulk containers, dry and wet mixers, cyclones, housings, loading areas. In addition suitable as vibration or insulation protection of machines.	WEICON Urethane 45, 60, 80 (Germany) (Weicon, 2009) Urethane 45 and 60 with phenylmercury neodecanoate, catalyst of Urethane 80 not indicated
Clear polyurethane compound for use on decals, labels, emblems and other decorated substrates	Z-8200 (U.S.A) (Development Associates, 2009)
Self-levelling sealants for penetration into joints of concrete flooring.	Permaflex B Gun Grade (UK) (Permaban, 2009)
For the production of film or theatre props where a firm flexible urethane moulding is required such as reproduction of weapons, etc.	J-Foam 130 (UK) (Jacobson Chemicals, 2009)
Film and television props and special effects applications for embedding hairs and for creating skin effects; Soft encapsulant for low voltage electronic assemblies; Soft seals or gaskets; General purpose mouldmaking; Rubber use as a mould backing material for silicone mould liners where a soft silicone requires firm but flexible support; Wear resistant coating for polyurethane foam and as a general purpose coating or repair system for items such as buoys fenders and conveyor belts. Electronic encapsulation and modelling display applications. Artistic and modelling display applications	E1105, E1118, XE1013, E106, E053 XR3002, XR3006 (UK) (Polymed, 2009) Indicated as “organic mercury catalyst”

Other applications mentioned by suppliers are different rollers of hard PU elastomers used for different applications, among these, rollers for swivel chairs and roller skates.

No specific confirmation of the current use of the mercury catalysts for flooring (discussed later under exposure) has been available; however, data sheets have been available for a few of the PU systems only. The application range is probably wider than indicated in the table above.

For many of the applications listed in the table above mercury-free alternatives exist. As many different PU elastomer systems exist, each used for production of different products, it has not been possible to obtain information on the breakdown of the total use into the different product groups. The mercury-based products are used both for the professional market and for consumer products.

According to a major manufacturer of PU catalysts, PU elastomer systems with aliphatic isocyanates is one of the areas where it has been difficult to replace mercury catalysts although the manufacturer estimate that substitution may be possible within a period of 3-5 years (discussed later).

According to the trade organisation ALIPA, polyurethanes based on aliphatic isocyanates are present in most of the high quality, long lasting coatings used in a wide number of applications such as (ALIPA, 2009):

- Automotive coatings, applied both as original equipment (OEM) and in car repair. Transportation applications such as aerospace, railway equipment, trucks and buses.
- Agricultural, construction and earth moving machinery.
- Plastic articles and components: bumpers, wheel covers, rear mirrors, door handles as well as phones, computers, skis, hifi equipment, kitchen ware.
- Wood Coatings: parquet flooring, heavy duty and high quality furniture for kitchen, school, counters.
- Maintenance & Protection Coatings: heavy industry anticorrosion (metallic structures), high performance decorative finishes.
- Marine: superstructure, topsides and decks of ships and yachts.
- Coil & Can Coatings: buildings (cladding and roofing), appliances, transport, packaging.
- General Industry: motorcycles, bicycles, metal office furniture.

Industry contacts have pointed out that mercury catalysts are widely used in the UK, Spain and Italy; relatively little used in Germany, although the overall industrial output is very high; while France is somewhere in the middle (COWI and Concorde East/West, 2008). Other EU countries do significantly less PU elastomer processing. Kometani *et al*. (year not indicated) from the Japanese chemical company Tosoh Corporation report, that although mercury catalysts are highly toxic and not used in Japan, Europeans and Americans continue to formulate using these catalysts. SPIN is a database on the use of substances and substances in mixtures in the Nordic countries. According to the SPIN database the compound was registered in 5 mixtures in Denmark in 2007 within the use category “construction materials” with a total indicated tonnage of 0. No use is registered for the other Nordic countries.

The catalysts are used for the manufacturing of different PU elastomer systems by manufacturers of plastic raw material systems like Dow Hyperlast, Baxenden Chemicals, Weicon and Belzona International. An Internet search reveals a large number of different systems with phenylmercury neodecanoate. Based upon a detailed investigation of the UK situation, COWI and Concorde East/West (2008) estimated that some 30-45 different mercury containing PU elastomer systems were marketed in the UK and at the EU level, recognizing that many systems are marketed in more than one EU country, they estimated that there may be as many as 200-250 different mercury containing PU elastomer systems. The total number of companies applying the mercury-containing PU systems is not known but likely several thousands. One of the areas, where mercury catalyst is widely used, is PU elastomers based on aliphatic isocyanates. According to the trade organisation ALIPA, for this particular market area, three companies were involved in the production of the chemical raw materials, 140 companies were involved in manufacturing of two-component systems while the number of end-use applicators was 2 200 (ALIPA, 2006).

Phenylmercury acetate
Phenylmercury acetate has traditionally been widely used as a biocide, plant protection product and as a catalyst in the production of polymers.

COWI and Concorde East/West (2008) report that 2.0 tonnes phenylmercury acetate were used in Italy in 2006 as biocide in the manufacturing of paints. They further report that suppliers inform that the consumption of phenylmercury acetate for fungal control and catalyst for polyurethane production is in the order of >15 tonnes. Slovenia (as quoted by COWI and Concorde East/West, 2008) reported that about 5 tonnes mercury are used for production of mercury compounds in the country, especially mercuric chloride, mercuric oxide and phenylmercuric acetate. For this study it has been reported by the Ministry of Health in Slovenia that phenylmercury acetate is not produced within the country.

As the mercury containing biocides are not included in the Review Programme under the Biocide Directive they should have been phased out by September 2006 and the mercury containing biocides are no longer lawfully on the European market. It has not been possible to confirm any current use of phenylmercury acetate as a biocide.

Phenylmercury acetate has traditionally been used as fungicides in agriculture, particularly for seed dressing (FAO, 1971). The use of pesticides based on phenylmercury acetate is not permitted in the EU and no uses are expected.

According to SPIN, the database on substances and substances in mixtures in the Nordic countries, phenylmercury acetate was in 2007 registered in 4 mixtures under the code "other colouring agents".

Phenylmercury acetate has previously been widely used as a catalyst for PU elastomers e.g. for sports tracks and floors as discussed in the literature about mercury releases from floors in Section B.9.3.2. It has not been possible to obtain any confirmation of such current uses in the EU + EFTA and industry contacts have indicated that it - to their knowledge - is not used.

The only indication of the current use of phenylmercury acetate as catalyst is the use as catalyst in a hardener, HW 8685 for a PU system from Huntsman Advanced Materials Americas Inc (U.S.A) (Huntsman, 2006). Mercury compounds have been used for the company's Araldite© PU adhesives, but the company announced in 2006 a family of mercury-free Araldite© polyurethane adhesives (ThomasNet, 2006). Is has not been investigated whether some adhesives from Huntsman still contain phenylmercury acetate and to what extent these may be used in the EU or EFTA.

It has only been possible to confirm the use of phenylmercury acetate for laboratory use. No information has been obtained on the total use. It is estimated that the current use is most probably <1 tonnes/year, but it cannot be ruled out that some illegal use of the substance as a biocide still takes place.

Phenylmercury 2-ethylhexanoate
Phenylmercury 2-ethylhexanoate is produced in significant quantities in the EU, but the substance is according to information from market actors nearly 100% exported.

Only one European supplier of phenylmercury 2-ethylhexanoate has been identified and the supplier has informed that the substance is supplied in small quantities for laboratory use only.

The substance is a well-known pesticide/biocide and the use of the compound is by COWI and Concorde East/West (2008) indicated as "bactericide, fungicide in paints". According to the questionnaire response from Italy for the study 4.4 tonnes phenylmercury 2-ethylhexanoate was used as biocide in the production of paint in Italy in 2006 (COWI and Concorde East/West, 2008). As the mercury containing biocides are not included in the Review Programme under the Biocide Directive they should have been phased out by September 2006 and the mercury containing biocides are no longer lawfully on the European market. It has not been possible to confirm any current use of phenylmercury 2-ethylhexanoate as a biocide in the EU+EFTA.

No details about the specific use of the phenylmercury 2-ethylhexanoate have been obtained.

The CAS No has been identified in a Material Safety Data Sheet (MSDS) from 1989 for a polyurethane system manufactured in the USA (CONAP, 1989). In the MSDS the name is indicated as phenylmercuric oleate. The product is not marketed anymore.

According to a supplier of "phenylmercury octoate" (CAS number not indicated) the total current EU consumption is probably in the order of a few hundred kg, but the consumption has been significantly higher formerly. The compound indicated as phenylmercury octoate may actually be phenylmercury 2-ethylhexoate or phenylmercury octanoate (both having 8 C atoms). The information in COWI and Concorde East/West (2008) concerning the application of "phenylmercury octoate" as catalyst is based on the same information source. One industry contact used the term "phenylmercury octoate" for phenylmercury neodecanoate, and there seems to be some confusion about the use of the term.

The SPIN Database on substances and substances in mixtures in the Nordic countries does not include any information on the compound.

Considering the information obtained from manufactures and suppliers it is estimated that the lawfully use of phenylmercury 2-ethylhexanoate in the EU+EFTA is most probably < 1 tonne/year.

Phenylmercury octanoate

It has not been possible to identify any information on current use of phenylmercury octanoate.

The substance is not included in the European chemical Substances Information System (ESIS) database or the list of substances pre-registered by ECHA, indicating that the substance is currently not used in the EU.

The SPIN Database on substances and substances in mixtures in Nordic countries does not include any information on the compound (SPIN, 2009).

As discussed above there is some confusion about the use of a substances indicated as "phenylmercury octoate" which may actually be phenylmercury 2-ethylhexoate or phenylmercury octanoate.

The substance is included in Pesticide Action Network (PAN) North America's Pesticide Database as "fungicide, microbiocide, herbicide" (PAN, 2009)

Considering the information obtained from manufactures and suppliers it is estimated that the use of phenylmercury octanoate in the EU+EFTA is most probably ~ 0 tonne/year.

Phenylmercury propionate

Phenylmercury propionate has according to a number of older patent applications conventionally been used as polyurethane catalyst (e.g. U.S. Patent, 1988). Requests to producers and suppliers of mercury chemicals and catalysts for polyurethane production, as well as a detailed search on the Internet, have not revealed any current use of phenylmercury propionate.

The SPIN Database on substances and substances in mixtures in the Nordic countries does not indicate any use of the compound in the Nordic countries.

The substance is included in Pesticide Action Network (PAN) North America's Pesticide Database as "fungicide, microbiocide, herbicide" (PAN, 2009)

Considering the information obtained from manufactures and suppliers it is estimated that the use of phenylmercury propionate in the EU+EFTA is most probably ~ 0 tonne/year.

B.2.3 Expected future use - baseline

Current manufacture, trade and use are shown in Table B-1. With regard to predicting future use of the substances, it is assumed that use of the mercury compounds 10 years ago was 2-3 times greater than current levels.

The consultation undertaken for the current analysis (see Section B.2 and C), indicates that there are significant ongoing efforts and pressures to further replace mercury-based catalysts in polyurethane products. However, no comprehensive data are available on the likely pace of future decline in use of the substances.

Whilst there is significant uncertainty in the rate of decline, it seems clear that there will continue to be a decline in use. However, it also seems clear that there are some uses of these compounds that will require additional time and effort if their replacement is to be achieved. Therefore, it is unlikely that these substances will be fully replaced by alternatives in the short to medium term without any additional regulatory pressure.

As such, for the purposes of this analysis, it has been assumed that use will continue to decline in the coming years but that use will not decline to zero over the timeframe of the analysis. The decline in use is therefore assumed to follow an exponential path, based on the historical decline.

An alternative scenario, assuming that manufacture, use and releases of the phenylmercury compounds would continue at current levels, was also considered within the assessment. However, this is not presented here because a continuation of current levels of use is not consistent with the information from consultation for this assessment, which clearly suggests declining levels of use.

A refinement could be to split the precedent exponential decay model into two components in order to better taking into account the 30% applications for which substitution will be difficult (lower exponential decay rate for these 30%). This would then increase the predicted volumes. So the predictions proposed hereafter based on a unique exponential decay rate shouldn't be considered as worst-case but rather as the minimum volumes that may be used if no restriction is applied.

Taking phenylmercury neodecanoate as an example, use in 2008 was estimated at 36-70 tonnes. Assuming that use 10 years previously was 2.5 times greater (i.e. the midpoint of 2 to 3 times greater), this corresponds to 90-175 tonnes. Therefore, the use profile is assumed to be as follows (the highlighted in yellow and orange values are the known and proposed ones, whereas the other values are modeled with an exponential decay rate estimated equal to 0.092):

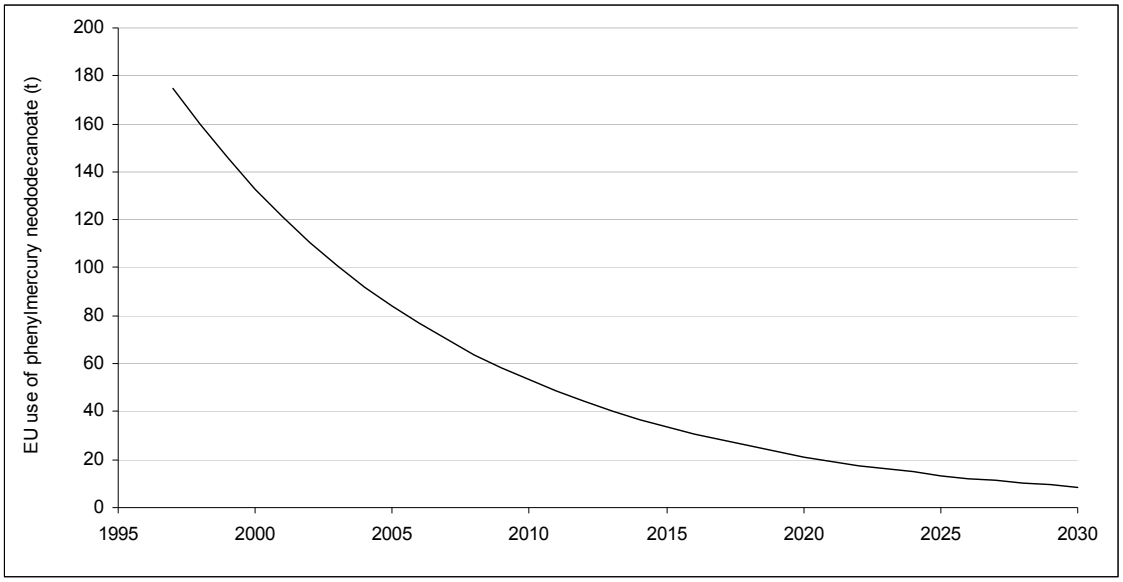
Table B-3 Expected use profile

Year	Use	
	High	Low
1998	175	90
1999	160	82

2000	146	75
2001	133	68
2002	121	62
2003	111	57
2004	101	52
2005	92	47
2006	84	43
2007	77	39
2008	70	36
2009	64	33
2010	58	30
2011	53	27
2012	49	25
2013	44	23
2014	40	21
2015	37	19
2016	34	17
2017	31	16
2018	28	14
2019	26	13
2020	23	12
2021	21	11
2022	19	10
2023	18	9
2024	16	8
2025	15	8
2026	13	7
2027	12	6
2028	11	6
2029	10	5
2030	9	5

Calculations are included in Appendix 11.

A graphic illustration of the same (assuming use at the upper end of the range given), gives the following figure:



Note: Assumes higher level of the range (36-70t) of use in 2008 and assumes use 10 years previously was 2.5 times higher (range given is 2-3 times higher).

Figure B.2-1 Illustration of assumed future use of phenylmercury neodecanoate

It is assumed that the export will follow the same downward sloping baseline as use in the EU.

B.2.4 Life-cycle manufacture and use of the phenylmercury compounds

Detailed information on all of the specific uses of these substances (in terms of final end products) was not possible to obtain for this study. Figure B.2-2 highlights the EU manufacture and main current uses.

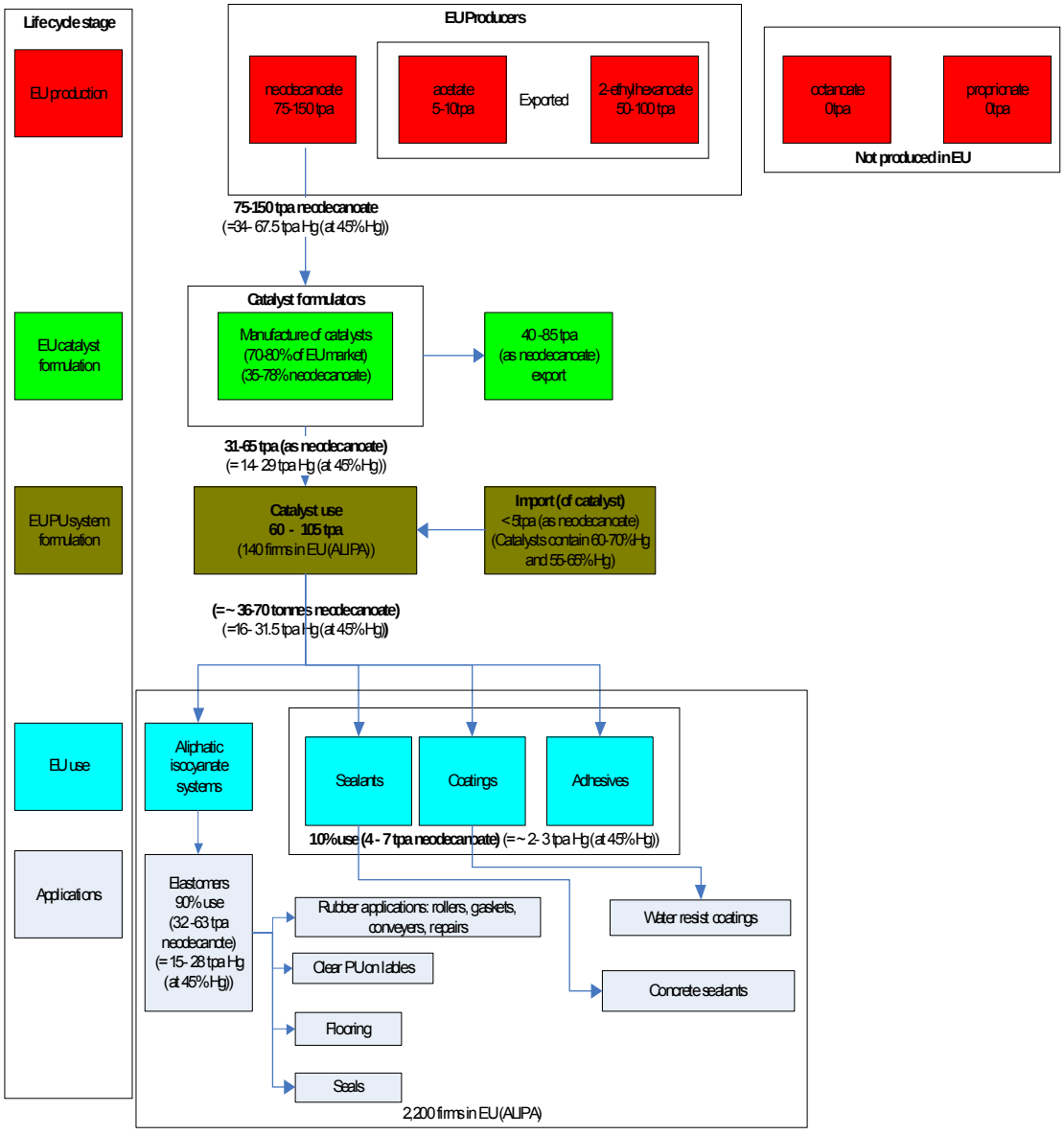


Figure B.2-2 Life-cycle manufacture and use of the phenylmercury compounds

B.2.5 Uses advised against by the registrants

No information available. Registration and submission of industry Chemical Safety Report (CSR) on the phenylmercury substances are, according to information from consultation for this study, envisaged in 2018.

B.2.6 Description of targeting

The concerns regarding the proposal for restrictions on the phenylmercury substances are related to both the environment and health.

B.3 Classification and labelling

B.3.1 Classification and labelling in Annex VI of Regulation (EC) No 1272/2008 (CLP Regulation)

An overview of the classification of the five phenylmercury substances, mercury and methylmercury according to Annex VI of Regulation (EC) No 1272/2008 (CLP Regulation) are presented in Table B-4 See Appendix 7 for details of the classification of the substances according to Annex VI of Regulation (EC) No 1272/2008 (CLP Regulation) and Annex I of Directive 67/548/EEC.

Table B-4 Classification and labeling according to CLP Regulation including 1st ATP from Annex I of the Regulation (EC) 790/2009

Phenylmercury acetate (CAS 62-38-4)	Acute Tox. 3 (oral) H301	Skin Corr. 1B H314	STOT RE 1 H372				Aq. Acute 1 H400	Aq. Chro. 1 H410
Index 080-004-00-7 Organic compounds of mercury with the exception of those specified elsewhere in this Annex **Phenylmercury propionate** (103-27-5) **Phenylmercury 2-ethylhexanoate** (13302-00-6) **Phenylmercury octanoate** (13864-38-5) **Phenylmercury neodecanoate** (26545-49-3)	Acute Tox. 1 (dermal) Acute Tox. 2 (oral) Acute Tox. 2 (inhal.) H330, H310, H300		STOT RE 2 H373				Aq. Acute 1 H400	Aq. Chro. 1 H410
Mercury (7439-97-6)	Acute Tox. 2 (inhal.) H330		STOT RE 1 H372			REPR. 1B H360D	Aq. Acute 1 H400	Aq. Chro. 1 H410
Methylmercury (22967-92-6)*	Acute Tox. 1 (dermal) Acute Tox. 2 (oral) Acute Tox. 2 (inhal.) H330, H310, H300		STOT RE 1 H372	MUTA. 2 H341	CARC. 2 H351	REPR. 1A Lact H360D, H361f, H362	Aq. Acute 1 H400	Aq. Chro. 1 H410

*Concluded by TC C&L, not adopted. Classification translated from DSD classification

B.3.2 Classification and labelling in classification and labelling inventory/ Industry's self classification(s) and labelling

No data found on industries self classification for the five phenylmercury compounds

B.4 Environmental fate properties

B.4.1 Degradation

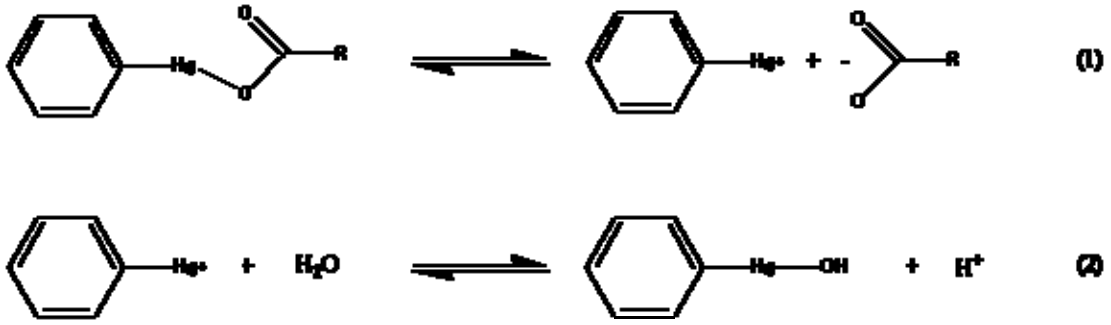
B.4.1.1 Abiotic degradation

B.4.1.1.1 Hydrolysis

Depending on the issue in discussion, phenylmercury(II) carboxylates have been described as molecules, complexes or salts. An aqueous solution of phenylmercury acetate will in part dissociate in phenylmercury cations and acetate anions justifying the term "salt" (Parikh and Sweet, 1961). On the other hand, phenylmercury acetate has a measurable vapour pressure at ambient temperatures which is normally associated with covalently bonded molecules (Lindström, 1958; Phillips *et al*., 1959).

Quantum-chemical analyses performed by Tang and Nielsen (2010) (see Appendix 12) reveal that phenylmercury carboxylates (acetate, propionate, 2-ethylhexanoate, octanoate and neodecanoate) can be regarded as compounds with primarily ionic character. The calculations indicate that the bonding around the Hg atom is independent of the nature of the carboxylate anion. This conclusion is drawn due to the fact that there is no systematic change in the net charge on the Hg and the interacting atoms, which is also reflected in the NMR shielding constants for the atoms in question.

Phenylmercury carboxylates dissolved in water will partly undergo dissociation into a carboxylate anion and a phenylmercury cation, which both will enter into equilibrium with their corresponding acids and bases (Parikh and Sweet, 1961). The phenylmercury carboxylates dissociate into a phenylmercury cation and a carboxylate according to reaction (1). The equilibrium of this reaction lies towards the undissociated molecule (left side of the equation). However, the phenylmercury cation reacts rapidly with water (hydrolyze) to form phenylmercury hydroxide (2). This reaction will drive the equilibrium of reaction (1) towards the phenylmercury cation.



R: acetate, propionate, 2-ethylhexanoate, octanoate or neodecanoate

Reaction (2) is pH-dependent and will not occur to a significant extent in acidic water (pH < 3-4) (Baughman *et al*., 1973, Klimisch Code: 1). However, within pH ranges usually found in natural waters (pH 5-9), the ions are almost completely hydrolyzed (Figure B.4-1) (Baughman *et al*, 1973, Klimisch Code: 1). At pH 4.2 50% of the phenylmercury species is dissociated. However, percentages of dissociated and undissociated compound change rapidly with

changing pH. At pH 3.2, 10% of the phenylmercury species is undissociated while at pH 5.1, 90% is undissociated.

Hydrolysis according to this reaction pattern is reported for phenylmercury acetate in Tomlin (1997) (Klimisch Code: 4) and Royal Society of Chemistry, (1983) (Klimisch Code: 4).

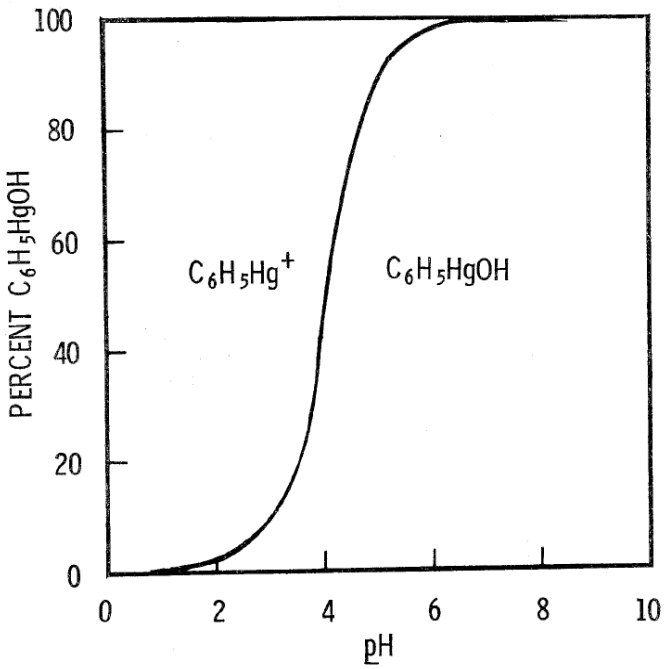


Figure B.4-1 pH dependence of the hydrolysis of phenylmercury ion. K = 6.8 · 10-5 (Baughman *et al.*, 1973)

Based on the rationale above it can be concluded that phenylmercury acetate, propionate, 2-ethylhexanoate, octanoate and neodecanoate dissociate in natural waters, soils and sediments (with pH-values between 5 and 9) and form the common compound phenylmercury hydroxide. For these environments, degradation of the five phenylmercury compounds can be assessed in the same way. Only in strongly acidic environments below pH 4, the phenylmercury carboxylates exist as undissociated molecules.

B.4.1.1.2 Phototransformation/photolysis

B.4.1.1.2.1 Phototransformation in air

Direct photolysis

Since tropospheric solar radiation has negligible intensity at wavelengths less than about 290 nm, phenylmercury acetate must have appreciable absorptivity at wavelengths greater than 290 nm if significant photoreaction is to occur in sunlight. Spectroscopic studies showed that phenylmercuric hydroxide, phenylmercury ion, and diphenylmercury absorb at wavelengths

> 290 nm (Baughman *et al*., 1973).Klimish Code:1- reliable without restrictions).

This result strongly indicates that phenylmercury acetate can be degraded by direct photolysis. Baughman *et al*. (1973) present an empirical photolysis half-life of phenylmercury acetate of t½ = 16 ± 2 hours (corresponding to a mean photolysis lifetime τ = 23 hours).

Baughman *et al*. (1973) cite studies published by Takehara *et al*.(1966) that report extensive photodecomposition of several phenylmercury compounds by sunlight. Photoreaction was more rapid when the compounds were dissolved in water than when they were irradiated as pure solids or in dust formulations. Major products from photolysis of phenylmercury acetate were reported to be Hg2O.

Also Zepp *et al*. (1973) report direct photolysis of phenylmercury acetate by cleavage of the phenyl-mercury bond resulting in a phenyl radical and a mercury-acetate cation (Hg+OCOCH3). Subsequently this can form a dimer molecule (i.e. (Hg OCOCH3)2) (Zepp *et al*., 1973). (Klimisch Code: 1-2 - Not guideline study, but reasonably well documented scientific study).

No data is available for the other four phenylmercury carboxylates. Therefore Tang and Nielsen (2010) calculated the vertical excitation energy of the five phenylmercury carboxylates in order to compare the photolysis activity. Based on the quantum chemical calculations all five compounds absorb light at wavelength of 330 nm and can therefore be degraded by direct photolysis in sunlight.

Photooxidation

The literature is scarce on atmospheric gas phase reactions of organomercury compounds.

The rate constant for the vapour-phase reaction of phenylmercury acetate with photochemically produced hydroxyl radicals has been estimated to be $2x10^{-12}$ cm^3/(molecule sec) at 25 °C using a structure estimation method. This corresponds to an atmospheric half-life of about 8 days at an atmospheric concentration of $5x10^5$ hydroxyl radicals per cm^3. (HSDB referring to Meylan and Howard, 1993, Klimisch Code: 4 - however, HSDB is generally considered to be a reliable database).

The estimation of the atmospheric half-life is based on the estimation software AOPWin, which is part of the EpiSuite™ (see Appendix 2). Dimethylmercury was part of the trainingsset when validating the software.

However, Tang and Nielsen (2010) pointed out that AOPWin does not include displacement reactions when estimating the atmospheric degradation of organomercurials (dimethylmercury and a series of phenylmercury carboxylates). However, this reaction is predominantly responsible for the photooxidation of organomercurials. Therefore, AOPWIN might underestimate the photooxidation activity of phenylmercury carboxylates and overestimate atmospheric lifetimes.

Tang and Nielsen (2010) assume that OH and NO_3 radicals react with phenylmercury carboxylates in displacement reactions (electrophilic attack) at the Hg atom where either the phenylring or the carboxylate rest is substituted.

$$\bullet OH + C_6H_5HgOC(O)CH_3 \rightarrow C_6H_5HgOH + \bullet OC(O)CH_3 \quad (3)$$

$$\rightarrow C_6H_5\bullet + CH_3C(O)OHgOH \quad (4)$$

Both processes will occur, but the reaction (4) will dominate.

The quantum chemical calculations of Tang and Nielsen (2010) indicate that other radical reactions like aliphatic H-abstraction (at the carboxylate) or addition to the phenylring are much slower than displacement reactions at the Hg atom and can be neglected for phenylmercury carboxylates (see Table B-5).

Table B-5 presents the estimated NO_3 and OH rate constants for their reactions with the five phenylmercury carboxylates. Calculations were conducted using the correlation between rate constants and ionisation potential and correcting for the offset of organomercurials. The rate constants increase with increasing chain length of the carboxylate rest, and it can be concluded that atmospheric life times decrease (to a small extent) from phenylmercury acetate via propionate, octanoate to 2-ethylhexanoate.

Table B-5 Estimated NO3 and OH rate constants for their reactions with the five phenylmercury carboxylates

Molecule	$k_{OH,displ.}$	$k_{OH,add.\ to\ phenyl\ ring}$	$k_{OH,H\text{-}abstr.\ from\ carboxylate}$	$k_{OH,tot}$	k_{NO3}
	$\cdot 10^{-12}$ cm^3 molecule^{-1} s^{-1}	$\cdot 10^{-12}$ cm^3 molecule^{-1} s^{-1}	$\cdot 10^{-12}$ cm^3 molecule^{-1} s^{-1}	$\cdot 10^{-12}$ cm^3 molecule^{-1} s^{-1}	$\cdot 10^{-15}$ cm^3 molecule^{-1} s^{-1}
Dimethylmercury	19.0			19.0	87
Phenylmercury acetate	17.1	1.9	0.04	19.0	55
Phenylmercury propionate	17.5	1.9	0.5	19.9	61
Phenylmercury 2-ethylhexanoate	25.4	1.9	6.3	33.6	313
Phenylmercury octanoate	23.7	1.9	7.3	32.9	230
Phenylmercury neodecanoate	Not calculated	1.9	6.5		Not calculated

Assuming a 24-hour average OH concentration of 5 x 10^5 cm^{-3} and a 12 hour night time NO_3 concentration at 1 x 10^9 cm^{-3}, Tang and Nielsen (2010) estimate lifetimes for reactions with OH radicals to $\tau_{OH} \approx 55$ hours, lifetimes for reactions with NO_3 radicals to $\tau_{NO3} \approx 14$ hours, and photolysis lifetime of $\tau_{photol} \approx 23$ hours. In conclusion, the average atmospheric lifetime of gaseous phenylmercury carboxylates is around 1 day.

Due to the low vapour pressure of the phenylmercury compounds, photolysis and photooxidation in air will mainly occur on surfaces and particles that are exposed to sunlight or at elevated temperatures.

Phototransformation of degradation products of phenylmercury compounds
In aquatic and terrestrial environments, phenylmercury compounds are degraded to various organic and inorganic mercury compounds. Of these, mainly elemental mercury, diphenylmercury and dimethylmercury are expected to be found in the atmosphere, due to elemental mercury's and dimethylmercury's high vapor pressure (0.002 and 50 mm Hg at 20 ºC, (Wilmarth and Rosencrance, 2003) and diphenylmercury's fairly low boiling point (204°C) and low water solubility (CRC Handbook, 1997). Other degradation products of phenylmercury acetate are not expected to be found in the atmosphere due to their rather ionic character.

Dimethylmercury does not absorb at wavelengths longer than 290 nm and will therefore not undergo photolysis in the stratosphere. However, OH and NO_3 radicals are able to degrade dimethylmercury in displacement reactions as Tang and Nielsen (2010) show. Rate constants for these reactions are presented in Table B-5.

Assuming a 24-hour average OH concentration of 5 x 10^5 cm^{-3} and a 12 hour night time NO_3 concentration at 1 x 10^9 cm^{-3}, lifetimes for reactions of dimethylmercury with OH radicals are estimated to $\tau_{OH} \approx 29$ hours, lifetimes for reactions with NO_3 radicals to $\tau_{NO3} \approx 3.2$ hours. Therefore, it can be assumed that dimethylmercury is easily degraded to either methylmercury or elemental mercury in the atmosphere.

Elemental mercury (Hg^0) is oxidized primarily by O_3, OH and NO_3 radicals to divalent mercury (Hg^{2+}) via either gas-phase reactions or aqueous-phase reactions in clouds and fog (Schroeder *et al*., 1991; Seigneur *et al*., 1994 as cited in Stein *et al*., 1996, Sommar *et al*., 1997, Sommar *et al*. 2001 as cited in Gårdfeldt *et al*., 2001). Hg^{2+} can complex with other ions, primarily chlorine, to form $HgCI_2$. Mercury deposits to water and soil, where it is oxidized to Hg^{2+}.

Methylmercuric chloride, methylmercuric hydroxide, and methylmercuric ion were not decomposed by direct photolysis in sunlight. Methyl mercury species are readily degraded by OH radicals but not by O_3 in the aqueous phase (Hoigne and Bader, 1978; Munthe, 1992 as cited in Gårdfeldt *et al*., 2001). As suggested by Tang and Nielsen (2010) photolysis lifetime of organomercurials in the gas phase will be very similar to or shorter than that of the aqueous phase. Therefore, results of photolysis experiments in pure water can be regarded as conservative estimates for the airphase.

B.4.1.1.2.2 Phototransformation in water

Phenylmercury acetate
The experimental half-life for direct photolysis of phenylmercury acetate in distilled water was found to be 16 hours when irradiated with Georgia, U.S. sunlight at a shallow depth. Using acetone as a photosensitizer, a disappearance quantum yield of 0.23 was reported. However, photosensitization is believed to be of little importance in the environment where the concentrations of the substance are low. Products from direct photolysis arise from the cleavage of the phenyl-mercurial bond and include metallic mercury, mercury(II) salts and products formed from reactions of the phenyl radical (Zepp *et al*., 1973). (Klimisch Code: 1-2 - Not guideline study, but reasonably well documented scientific study).

The predicted half-life for the photolysis of phenylmercury acetate in near-surface water during midsummer at 40 ºN latitude is 1.6 days (Zepp and Baughman, 1978). (Klimisch Code: 4 - Not experimental study, but good quality predictive modelling study based on experimental data (no details in paper) and theoretical considerations).

In water, 75% of phenylmercury acetate was recovered after 10 hours of sunlight irradiation. The only identified phenylmercury acetate photolysis product was mercurous oxide (Crosby and Li, 1969). (Klimisch Code: 4 - comprehensive review).

According to Baughman *et al*. (1973), the rate of sunlight absorption is pH-independent. To determine empirically the effect of materials dissolved in natural waters on the quantum yield for photodecomposition of a phenylmercuric salt, air-saturated solutions of phenylmercury acetate (1.0×10^{-3} M) in two different natural waters and in distilled water were subjected to equal exposures of Pyrex-filtered mercury-lamp light (> 290 nm). The phenylmercuric salt photodecomposed at the same rate in all three solutions. Dark controls showed no decomposition.

Photolysis in water is expected to dominate in the surface near water layers where irradiation is highest. The water depth to which phenylmercury compounds can be photodegraded is mainly dependent on the presence of particles and dyes (especially humic substances).

Phenylmercury propionate, octanoate, 2-ethylhexanoate and neodecanoate
No data found. However, as the vertical excitation energies reported by Tang and Nielsen (2010) indicate, the propionate, octanoate, 2-ethylhexanoate and neodecanoate will behave in the same way as the phenylmercury acetate. Prior to photochemical reaction, the phenylmercury carboxylates dissociate into phenylmercury and the corresponding carboxylate. The phenylmercury (either present as cation or as hydroxide) can be further degraded by photolysis and radical mediated photooxidation. Reactions with radicals predominantly involve displacement reactions at the Hg atom where the molecule is cleaved between phenyl ring and Hg atom.

In water, dissociation or a competing hydrolysis reaction may be expected (which lead to formation of phenylmercury oxide or hydroxide). The hydrolysis product can be phototransformed (by cleavage of the phenyl-mercury bond) at about the same rate as the parent molecules (Zepp *et al*., 1973).

B.4.1.1.2.3 Phototransformation in soil

No data found.

B.4.1.2 Biodegradation

B.4.1.2.1 Biodegradation in water

Phenylmercury acetate

Phenylmercury acetate is a salt-like compound that easily dissociates in water to phenylmercury and acetate (the dissociation constant is similar to acetic acid) (Parikh & Sweet, 1961). A comparison of the infrared spectra of potassium acetate, phenylmercury acetate and methyl acetate conducted by Tang and Nielsen (2010) confirms this fact.

According to Baughman *et al*. (1973), more than 99% of the phenylmercury acetate is dissociated at concentrations below 10^{-7}M (33.74 µg/l) (see also chapter B.4.1.1.1). The resulting phenylmercury cation ($Ph\text{-}Hg^{+}$) or phenylmercury hydroxide (Ph-Hg-OH) are chemically more stable and are not split by water or weak acids or bases. They can, however, be degraded by microorganisms. Phenylmercury acetate is degraded by aquatic microorganisms to metallic mercury (Hg°) and benzene as Nelson *et al*. (1973) showed. According to this study, selected mercury tolerant bacterial species isolated from estuarine waters and sediments were capable to degrade 50-60% of phenylmercury acetate within 1 h. (Klimisch Code: 1-2 - No guideline study, but good scientific documentation of methods and results). The degradation is catalyzed by the enzyme organomercury lyase with divalent mercury (Hg2+), benzene and acetate as products (Mirgain *et al*., 1989). Divalent mercury can be transformed by the mercury reductase to metallic mercury or methylmercury.

Jernelöv (1969 as cited in Kumar, 2003) postulated based on experimental investigations that the transformation of phenylmercury compounds to methylmercury in the aquatic environment takes place via the divalent inorganic cation. (Klimisch Code: 4 - however, the experimental work by Jernelöv and Jensen & Jernelöv on mercury methylation and demethylation is referred to by several authors and has been regarded as "axiomatic" for many years (Miller, 1984 - Klimisch Code: 4).

Using a sewage sludge inoculum, phenylmercury acetate at an initial concentration of 5 and 10 mg/l was found to degrade to inorganic mercury compounds (not specified further) at a rate of 50% and 60% removal after 7 days, respectively. The delayed removal was not believed to be due to inhibitory concentrations of phenylmercury as a reference compound, formaldehyde, was degraded at normal rate in the experiment (Pauli and Franke, 1971). (Klimisch Code: 2 - reasonable resemblance with guideline method).

Phenylmercury propionate, octanoate, 2-ethylhexanoate and neodecanoate
No data found. However, at low concentrations (< 10-7 M or < 35 µg/l) and within pH ranges normally found in natural waters (pH 5 – 9), phenylmercury carboxylates are dissociated into phenylmercury and a carboxylate anion. With phenylmercury as common intermediate, it is considered likely that the propionate, octanoate, 2-ethylhexanoate and neodecanoate do not behave differently from the acetate with regard to biodegradation in water. At pH-values lower than 3.5, phenylmercury carboxylates are undossiciated. In this case, biodegradability of the compounds will be increasingly limited with increasing molecular weight due to reduced bioavailability of the compounds. However, in such environments biological life is already hampered by low pH-conditions.

Generally, it can be stated that all four substances will most likely be transformed to inorganic mercury species (divalent and/or monovalent cations or elemental mercury), which, under anaerobic conditions, can be biotransformed to methylmercury.

Environmental fate of degradation products
Inorganic mercury

When phenylmercury compounds are degraded to inorganic mercury (divalent and metallic mercury), inorganic mercury can be transformed to other mercury compounds according to the biogeochemical pathways described in Section B.4.1.3. In waters, divalent mercury can be chemically or microbiologically reduced to elemental mercury or microbiologically transformed to methylmercury or dimethylmercury. The latter process occurs predominantly at anaerobic conditions in deeper water layers near the sediment.

B.4.1.2.2 Biodegradation in sediments

Phenylmercury acetate
Phenylmercury acetate is quickly degraded in soil and by sediment living microorganisms, with diphenylmercury, benzene, divalent and metallic mercury as degradation products. At anaerobic conditions, methylmercury can be produced. Matsumura *et al*., (1971) showed that microorganisms isolated from natural lake sediment and from soil were capable to degrade all phenylmercury (0.67 ppm) at a temperature of 30 ºC within 10 days. They identified diphenylmercury as one of the main metabolites (Matsumura *et al*., 1971). (Klimisch Code: 1-2 - Not guideline study, but good quality scientific study).

Nelson *et al*. (1973) performed degradation experiment where cultures of mercury tolerant bacteria were isolated from water and sediment and exposed to 0.4 ppm phenylmercury acetate at 25ºC. The different cultures that predominantly consisted of Pseudomona strains degraded between 2 and 40% of phenylmercury acetate within 4 days. (Klimish Code: 1-2, scientifically sound and well described study)

The total mercury concentrations in sediments from 2 stations in Minamata Bay, Japan were 32.4 and 23.5 µg/ml, respectively. The minimum inhibitory concentrations of a number of mercury compounds against the strains volatilizing methylmercury were studied using the mentioned two sediments. The minimum inhibitory concentrations of mercury chloride and phenylmercury acetate were 80-160 and 4-8 µg/ml, respectively. However, at only 8 µg/ml the inhibitory effect of phenylmercury acetate exceeded 50%. All of the methylmercury-volatilizing bacteria were able to volatilize phenylmercury. The volatilization by such bacteria was found to be 44-45 % (Nakamura *et al*., 1988). (Klimisch Code: 2 - not guideline study, but experimental study of apparently acceptable quality).

Phenylmercury propionate, octanoate, 2-ethylhexanoate and neodecanoate
No data found. However, at low concentrations (< 10^{-7} M or < 35 µg/l) and in sediments with a pH value between 5 and 9, phenylmercury carboxylates are dissociated to phenylmercury and a carboxylate anion. With phenylmercury as common intermediate it is considered likely that the propionate, octanoate, 2-ethylhexanoate and neodecanoate do not behave differently from the acetate with regard to biodegradation in sediments.

Presumably, all four substances will eventually be completely transformed to inorganic mercury species (divalent and/or monovalent cations or elemental mercury), which, under anaerobic conditions, can be biotransformed to methylmercury.

Environmental fate of degradation products
Inorganic mercury

When phenylmercury compounds are degraded to inorganic mercury (divalent and metallic mercury) in sediments, inorganic mercury can be transformed to other mercury compounds according to the biogeochemical pathways described in Section B.4.1.3.

Diphenylmercury
In studies of Matsumara *et al*. (1971), diphenylmercury was identified as one of the main degradation products in sediments. Diphenylmercury is more hydrophobic than phenylmercury acetate with a log K_{OW}= 3.06 (estimated with EpiSuite 4.0, see Appendix 2) and a water solubility of 4.1 mg/l. The vapor pressure is estimated by EpiSuite 4.0 to 0.06 mm Hg (see Appendix 2), which is comparable with the vapour pressure of metallic mercury (Edmonds *et al*., 1996). Unlike the phenylmercury carboxylates, diphenylmercury does not dissociate in water. The high vapour pressure of diphenylmercury indicates high volatility of diphenylmercury. One might expect that diphenylmercury behaves like dimethylmercury, due to structural similarities. If so, a short atmospheric lifetime (1 day) (Sommar *et al*., 1996) should be expected due to the compound's instability towards photochemical dissociation. The metabolite would be phenylmercury which would quickly deposit due to its rather ionic character.

Due to the higher hydrophobicity, diphenylmercury is expected to sorb more strongly to organic matter than phenylmercury acetate.

B.4.1.2.3 Biodegradation in soil

Phenylmercury acetate
In most studies phenylmercury acetate is quickly degraded by soil microorganisms to divalent mercury, metallic mercury and diphenylmercury. The presence of noticeably concentrations of methylmercury in soil is restricted to anaerobic conditions where methylation of mercury may exceed demethylation rates.

Matsumura *et al*., (1971) identified diphenylmercury as one of the major metabolic products of phenylmercury acetate in a biodegradation experiment with isolated bacterial cultures from soils and sediments. After 10 days incubation at 30ºC, no phenylmercury acetate could be detected (Klimisch Code: 1-2 - Not guideline study, but good quality scientific study).

In soil and microbial cultures, phenylmercury acetate is transformed to benzene and metallic mercury, although specific details were not provided (Alexander 1981). (Klimisch Code: 4 - but considered to be a high quality review).

Large concentrations of phenylmercury acetate, 200 to 630 ppm, underwent rapid degradation in several different soils (Levi and Crafts, 1952 cf. HSDB). (Klimisch Code: 4 - however, HSDB is generally considered to be a reliable database).

Following 28 days of incubation in soil, 60-70 % of applied phenylmercury acetate was still present as phenylmercury in soil while approximately 14-16% were degraded to metallic mercury and had volatilised. (Kimura and Miller, 1964). (Klimisch Code: 2 - Not guideline study but well documented study with sound conclusions).

Hempel *et al*. (1995) studied the fate of phenylmercury in soil lysimeters. The results reveal that most of the phenylmercury is transformed to inorganic mercury and strongly bound to the soil. After 14 days, only 19% of the phenylmercury could be detected in soil.

Kimura and Miller (1964) showed that moisture in soil decreases the amount of evaporating mercury in phenylmercury acetate contaminated soils. The phenylmercury hydroxide strongly sorbs to particles and humic material (Capel *et al*., 1988).

Phenylmercury propionate, octanoate, 2-ethylhexanoate and neodecanoate
No data found. However, as the initial reaction in the environment appears to be dissociation of the compound in phenylmercury and a carboxylate anion, it is considered likely that the propionate, octanoate, 2-ethylhexanoate and neodecanoate salts of phenylmercury do not behave much differently from the acetate with regard to initial biodegradation in soil.

Presumably, all four substances will eventually be completely transformed to inorganic mercury species (divalent and/or monovalent cations or elemental mercury), which, under anaerobic conditions, can be biotransformed to methylmercury.

Phenylmercury compounds in landfills
The fate of phenylmercury compounds in landfills has not been studied. What is more, except from investigations focusing on the airborne emissions of mercury with landfill gas and leachate composition, no experimental data are available on the fate of mercury in municipal landfills. Therefore, considerations on the fate of mercury and specifically on phenylmercury carboxylates in landfills have to be based predominantly on observations in sediments and airborne emissions from landfills.

The fate of mercury in landfills is strongly related to redox and pH-conditions and their changes.

Generally, it is accepted that landfills undergo at least four phases of decomposition, (1) an initial aerobic phase, (2) an anaerobic acid phase, (3) an initial methanogenic phase, and (4) a stable methanogenic phase. Subsequent phases of decomposition, in which the waste cell begins to turn aerobic are based on theory. The initial aerobic phase in a landfill lasts only a short period because oxygen is not replenished once the waste is covered. As oxygen sources are depleted, the waste becomes anaerobic, which supports fermentation reactions. This process proceeds efficiently over a relatively narrow pH range around neutral. In the second phase the hydrolytic, fermentative, and acetogenic bacteria dominate, resulting in an accumulation of carboxylic acids, and a pH decrease (Kjeldsen *et al*., 2002). During the third, methanogenic phase, strongly reduced conditions dominate and the methane production rate increase. The pH increases and stabilizes around neutral to weakly basic.

Especially the environmental conditions in the aerobic (phase 1) and anaerobic acid phase (phase 2) with high microbiological activities and elevated temperatures are expected to stimulate degradation of polyurethane and phenylmercury carboxylates, as well as release of mercury from polyurethane. How far degradation proceeds is dependent on the type of polyurethane and on the surface-to-volume ratio of the polyurethane. Due to the buffering properties of organic acids in decomposed waste it can be assumed that the pH in the landfill does not drop below pH 4.5 (Kjeldsen *et al*., 2002). Therefore, phenylmercury carboxylates dissociate at these conditions to phenylmercury and a carboxylate. Phenylmercury compounds that are released from polyurethane are probably more easily degraded at aerobic

conditions than at anaerobic conditions. No information is available on the anaerobic degradation of phenylmercury compounds, however nonsubstituted phenols are generally more easily degraded at aerobic than at anaerobic conditions. Both microbiological and chemical degradation of phenylmercury compounds are expected to occur in landfills.

Phenylmercury compounds that are degraded to divalent mercury can be reduced to volatile elemental mercury in anoxic conditions and escape the landfill either through the landfill cover or through landfill gas flares. Emission of elemental mercury to air has been demonstrated in several investigations (Lindberg *et al*., 2005; Lindberg *et al*., 2004, Li *et al*. 2010, Kim *et al*., 2002). These studies also report elevated concentrations of methylmercury and dimethylmercury in landfill gas indicating that landfills act as bioreactors for methylated mercury compounds. Methylation of mercury to monomethylmercury and dimethylmercury is favoured at anaerobic conditions and high microbiological activities (Ullrich *et al*., 2002; Korthals and Winfrey, 1987; Pak and Bartha, 1998). The persistence of monomethylmercury is also highest under anaerobic conditions. Besides, acidic conditions are expected to increase the solubility of monomethylmercury (Ullrich *et al*., 2001). Highest production and release of methylmercury can therefore be expected in the second anaerobic, acid phase of a landfill. In this phase, redox conditions are moderately anaerobic and net production of methylmercury is expected to be highest (Ullrich *et al*., 2001). Under strongly reducing conditions, the production of methylmercury is expected to decrease due to the formation of (nearly) insoluble mercurysulphide (HgS). In strongly reducing environments sulphate is reduced to sulphide, the pH is weakly basic and divalent mercury precipitate as HgS. However, although MMHg production is generally greatly reduced at high sulfide concentrations, it is not usually completely inhibited (Ullrich *et al*., 2001). Furthermore, demethylation of methylmercury is considerably delayed at anaerobic conditions.

Ullrich *et al*. (2001) cite several studies that suggest the transformation of monomethylmercury to volatile dimethylmercury in the presence of high sulphide concentrations. The formation of dimethylmercury is considered a potentially important loss mechanism of monomethylmercury from landfills.

Release of mercury from landfills through landfill leachate is expected to occur predominantly in the acid anaerobic phase where high concentrations of dissolved organic matter facilitate the release of mercury out of the landfill (Kjeldsen *et al*., 2002). According to Kjeldsen *et al*. (2002b), mercury is found in rather low concentration in landfill leachate (between 0.05 and 160 µg/l), which makes this release pathway less important compared to atmospheric emissions.

Environmental fate of degradation products

Inorganic mercury

When phenylmercury compounds are degraded to inorganic mercury (divalent and metallic mercury) in sediments, inorganic mercury can be transformed to other mercury compounds according to the biogeochemical pathways described in Section B.4.1.3.

Diphenylmercury

See environmental fate of diphenylmercury in sediment, Secton B.4.1.2.2.

B.4.1.3 Summary and discussion on degradation

All five phenylmercury compounds (phenylmercury acetate, propionate, 2-ethylhexanoate, octanoate and neodecanoate) are salt-like compound substances that dissociate to phenylmercury and the corresponding carboxylate. More than 90% of the compound is dissociated in environments with a pH value between 5 and 9. At these pH values phenylmercury is mainly present as phenylmercury hydroxide. Dissociation of phenylmercury acetate is the initial reaction for the chemical and biological degradation of phenylmercury acetate.

Abiotic degradation of phenylmercury acetate occurs predominantly in air and upper layers of waters where it is degraded to divalent and metallic mercury by phototransformation. Based on quantum chemical calculations **atmospheric lifetimes were estimated to approximately 1 day**. Atmospheric lifetimes of the phenylmercury compounds are expected to decrease with increasing chain length of the carboxylate. Because of the low vapour pressure of the compounds photolysis and photooxidation in air are likely to occur on surfaces and particles where the compounds condensate. Dimethylmercury and diphenylmercury, possible volatile biodegradation products of phenylmercury carboxylates, are easily photodegraded to methylmercury and inorganic mercury in the atmosphere.

Photochemical degradation of phenylmercury carboxylates in water will predominantly occur in surface near water layers at half lives between 16 and 39 hours.

Available literature on the biodegradation of phenylmercury acetate shows that microorganisms are capable to cleave the phenyl-mercurial bond of phenylmercury. It is reported that phenylmercury acetate is rapidly degraded in waters by mercury tolerant microorganisms to metallic mercury and divalent mercury**. Half lives for degradation of the phenylmercury cation in waters are within hours to days**, however, the available data is based on experiments with bacterial cultures.

In sediments, phenylmercury carboxylates are expected to easily biodegrade within days and weeks. Published data indicate that half lives are below 6 weeks. Main degradation products are divalent mercury and metallic mercury. At anaerobic conditions methylmercury is formed. Volatile diphenylmercury is one of the main intermediate degradation products of phenylmercury acetate. However, all available data is based on experiments that were conducted at aerobic conditions. Anaerobic degradation of phenylmercury is expected to occur more slowly with metallic mercury and methylmercury as main degradation products. Diphenylmercury is moderately volatile and easily degraded in the atmosphere by photolytic degradation.

In soils, phenylmercury acetate is degraded to metallic mercury, divalent mercury and diphenylmercury. Transformation of divalent mercury to methylmercury and exposure of soil organisms is a less relevant process. **Degradation rates of phenylmercury acetate in soils differ between soils, and half lives ranging from some days to several weeks are reported.** The results of the cited studies indicate that the half life of phenylmercury acetate is probably lower than six weeks, but it cannot be ruled out that degradation occurs more slowly at colder climates and in soils with low microbial activity. Degradation is closely related to physical-chemical conditions in soil. High sorption capacity of soil retards degradation.

The degradation pathway of phenylmercury acetate in the aquatic and terrestrial environment is outlined in Figure B.4-2.

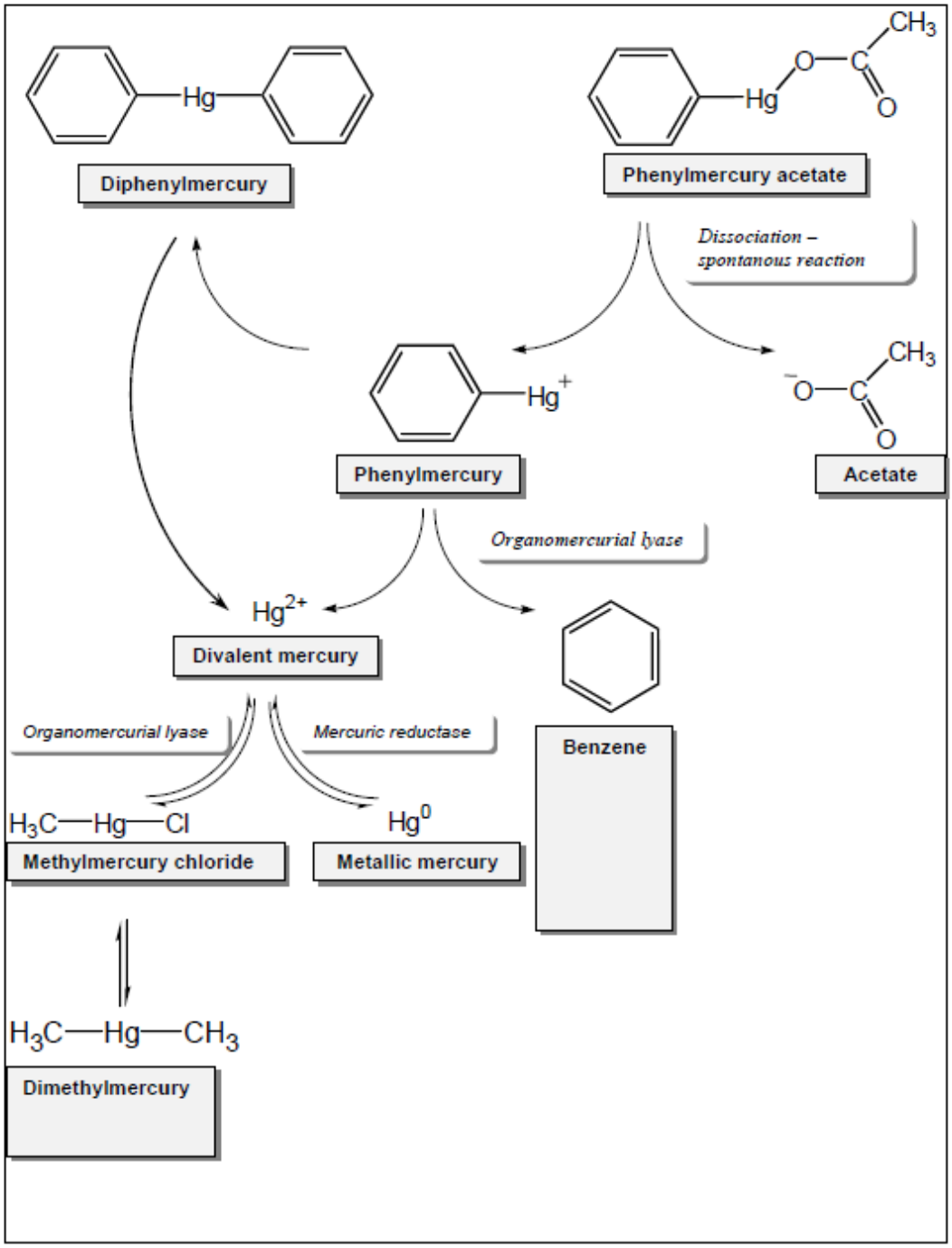


Figure B.4-2 Degradation pathway (simplified) of phenylmercury acetate in the aquatic and terrestrial environment. In upper water layers, photodegradation of phenylmercury acetate may occur abiotically.

The biogeochemical pathway of mercury

The primary form of mercury in the atmosphere is elemental mercury which may be oxidised to the mercuric ion form by photocatalytic reactions (Winfrey and Rudd, 1989). Mercurous (Hg^{+}) salts (e.g. mercurous chloride) are not very soluble in water and are therefore much less

bioavailable and toxic than the divalent mercuric forms (e.g. mercuric chloride, mercuric nitrate and mercury acetate) (Stretcher, 1968).

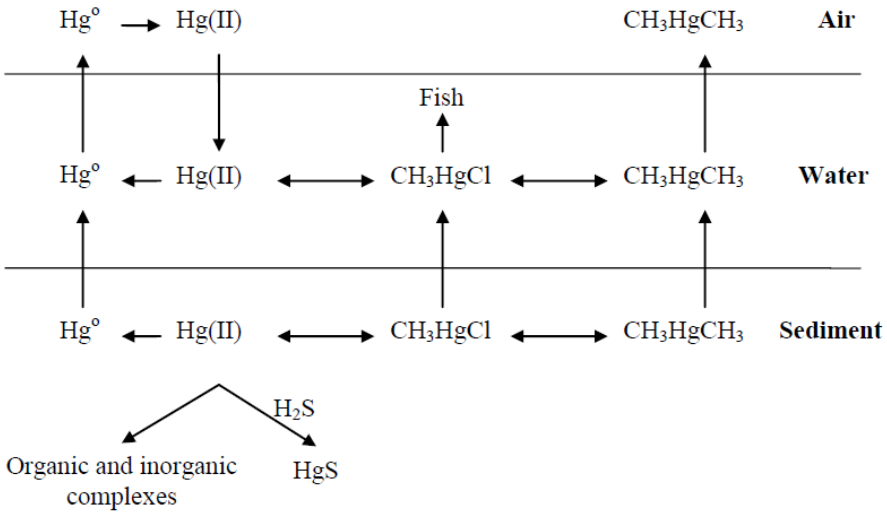
The cycling and distribution of mercury in the environment is mainly affected by methylation/demethylation processes, redox conditions, precipitation of insoluble mercury compounds, dissolution processes, and sorption/desorption processes. These processes often interact with each other forming a complex system of synergistic and antagonistic effects.

Once released to the atmosphere, Hg^0 can be transported over long distances. Reported lifetimes in the atmosphere are between 90 days and 2 years (Stein *et al*., 1996). In the atmosphere elemental mercury can be oxidized to divalent mercury via either photooxidation or aqueous-phase reactions in water droplets in air. This results in the deposition of mecury to water and soil. Once oxidized, divalent mercury can be methylated by microbes to methylmercury compounds. Notably monomethylmercury is absorbed by aquatic plants and animals and bioconcentrates up the food chain.

Dimethylmercury volatilizes to the air, where it photolyzes to methane, CO_2 and elemental mercury or is oxidized by hydroxyl or nitrate radicals. In strongly anaerobic environments and in the presence of complexing agents, mercury sulphide may form, which may represent a sink for mercury. However, under certain circumstances mercury sulphide can be resolubilized by bacterial transformation (Driscoll *et al*., 1994 as cited in Stein *et al*., 1996). According to Stein *et al*., (1996), the flux of mercury from the water and soil back into the air generally exceeds the deposition flux.

The biogeochemical cycling of mercury in freshwater (simplified) (adapted from Winfrey and Rudd, 1989) is shown in Figure B.4-3

Figure B.4-3 The biogeochemical cycling of mercury (simplified)



Hgo	Elemental mercury
Hg(II)	Inorganic mercury
CH3Hg+	Methylmercury
CH3HgCH3	Dimethylmercury
HgS	Mercuric sulphide
CH3HgCl	Methylmercurychloride

Phenylmercury compounds or other organomercury compounds may join this biogeochemical cycle after a first fast dissociation in phenylmercury cation which will in water rather be in the form of phenylmercury hydroxylate and then easily be transformed into elemental mercury or other mercury compounds of this cycle (seeFigure B.4-3 above and Appendix 12).

Inorganic mercury can be methylated abiotically or microbiologically, however, chemical methylation is less important than microbiologically mediated methylation (Ullrich *et al*., 2001). A prerequisite for the methylation of mercury is the presence and availability of divalent mercury. Inorganic mercury that readily adsorbs to inorganic and organic particulates including dissolved organic carbon, will not be available for methylation (Winfrey and Rudd, 1989). Divalent mercury is methylated predominantly under anaerobic conditions in sediments by sulphate reducing bacteria (Newman and Unger, 2003) and microorganisms that produce methane (Atlas and Barta, 1981). The methylation process produces monomethyl and dimethyl-mercury.

Although highest methylation activities are expected in moderately anaerobic surface sediments just below the sediment/water interface significant methylation of mercury also occur in anaerobic water layers and in the intestines and external slime layers of fish (Winfrey and Rudd, 1989). Methylmercury formed in the aquatic environment is biologically demethylated by microorganisms. Demethylation occurs under both aerobic and anaerobic conditions, although greater demethylation activity has been observed under aerobic conditions (Pak and Bartha, 1998; Korthals and Winfrey, 1987; Stein *et al*., 1996). Demethylation can be conducted by mercury resistant bacteria resulting in the formation of elemental mercury (Winfrey and Rudd, 1989).

According to Stein *et al*. (1996), biological demethylation occurs at a much lower rate than methylation. It is important to note that in the environment both methylation and demethylation processes occur and environmental concentrations of methylmercury reflect net methylation rather than actual rates of methylmercury production. It appears that the combined effect of methylmercury production and degradation leads to a state of equilibrium with a near constant level of methylmercury in sediments (Beijer and Jernelöv, 1979, Pak and Bartha, 1998 as cited in Ullrich *et al*., 2001) that rarely exceeds 1 to 1.5% of total mercury concentration whereas the proportion of methylmercury in fish and other aquatic biota may be much higher. Several factors such as pH, redox conditions, microbial activity, the amount of organic material, salinity and sulphide concentration influence the net production of methylmercury. However, these factors do not only affect biological methylation and demethylation rates, but also control sorption and solubility of the different mercury species.
Generally, it is believed that low pH increases the solubility of methylmercury resulting in higher bioaccumulation of methylmercury in biota. Moderatly anaerobic conditions that do not promote precipitation of mercury sulphide support the net production of methylmercury while aerobic and strongly reduced environments restrict methylation. It is also observed that the methylating activity of marine and estuarine sediments is usually lower than that of freshwater sediments (e.g., Olson and Cooper, 1974 Blum and Bartha, 1980, Compeau and Bartha, 1987 as cited in Ullrich *et al*., 2001), which generally has been attributed to salinity effects.

Methylmercury can be further methylated to volatile dimethylmercury primarily under alkaline conditions (Winfrey and Rudd, 1989). Methylmercury and dimethylmercury formation rates are of similar magnitude at 20°C. However, low pH values appear to favor the production of methylmercury, while dimethylmercury is predominantly formed under neutral

and basic (pH>7) conditions. A number of studies have suggested that in the presence of high sulfide concentrations, methylmercury may be converted to volatile dimethylmercury making dimethylmercury formation to a potential loss process for methylmercury from sediments (Craig and Bartlett, 1976, Craig and Moreton, 1984, Baldi *et al*.1995 as cited in Ullrich, 2001). Dimethylmercury is easily degraded to methylmercury. While the formation of dimethylmercury is microbiologically mediated, its degradation occurs chemically (Ullrich *et al*., 2001).

According to Weiner *et al* (2003) the methylation of mercury and subsequent exposure to methylmercury occurs predominantly in the aquatic environment. This microbial process exacerbate mercury toxicity because methylmercury is the most toxic and bioaccumulative form of mercury (Weiner *et al*., 2003).

Despite a vast body of literature on the subject, it is still not possible to predict Hg methylation rates and the likely effects of environmental changes on methylation and demethylation processes in aquatic systems (Ullrich *et al*., 2001).

B.4.2 Environmental distribution

B.4.2.1 Adsorption/desorption

Dissociation of all five phenylmercury carboxylates into the phenylmercury cation and the correspondent carboxylate enables strong sorption of the phenylmercury cation to clay and organic particles (Hogg *et al*. (1978), Aomine and Inoue (1967), Inoue and Aomine (1969), Dalland *et al*. (1986)). Dependent on the pH in soil phenylmercury is present as the phenylmercury cation or as phenylmercury hydroxide. In soil with pH 5 to 9 phenylmercury will predominantly be present as phenylmercury hydroxide, while divalent mercury is present as mercuric hydroxide ($Hg(OH)_2$ (Baughman *et al*., 1973)). At pH < 4, both the phenylmercury compounds are undissociated and the aromatic and aliphatic parts of the compounds are responsible for strong sorption to mainly organic material. In soils with pH > 4, phenylmercury occurs as an uncharged hydroxycomplex that mainly sorbs to mineral surfaces and organic matter by electrostatic and van-der-Waals forces and through surface complexation. Surface complexation of mercury to hydroxyligands at the mineral surfaces is described by Schuster (1991) and results in strong sorption of mercury hydroxide. A similar process can be expected by phenylmercury hydroxide that might form surface complexes with hydroxyligands at mineral surfaces.

Experimental data on sorption behaviour was solely found for phenylmercury acetate.

Sorption of phenylmercury acetate to inorganic soil colloids was found to be highest for montmorillonite, next allophone and lowest in kaolinite and was strongly affected by pH and ionic strength (Inoue and Aomine (1969)). Highest adsorption capacity was reported at pH 6. According to Hogg *et al*. (1978) and Dalland *et al*. (1986), however, organic colloids are more important for the sorption of phenylmercury acetate than inorganic colloids and explain differences in sorption between different soil types.

Dalland *et al*.(1986) investigated sorption of phenylmercury acetate to humic acid, iron and manganese oxides in seawater and found a ten times higher sorption coefficient to humic acids than to inorganic colloids. According to this study, the organic carbon normalized sorption coefficient (Koc) for phenylmercury acetate in seawater was calculated to 50,000 L/kg. (Klimisch Code: 2- reliable with restrictions).

Hogg *et al*. (1978) studied sorption of phenylmercury acetate in two soil types with different organic content. Sorption could be described by Langmuir isotherms, and sorption coefficients were derived from these Langmuir isotherms at low aqueous concentrations. The Koc of phenylmercury acetate varied between 3,164 and 8,333. (Klimisch Code: 2- reliable with restrictions).

The lower Koc in soil compared to organic colloids in saltwater is likely due to a salting out effect which reduces the solubility of organic compounds in water and increases sorption (Turner *et al*., 2001; Dalland *et al*., 1986).

In an environmental study of the river Rhine following a major accidental release of pollutants resulting from a fire at the Sandoz chemical company in Basel, Switzerland, it was found that the phenylmercury cation sorbed strongly to particles and humic material in the

water column. (Capel *et al*., 1988). (Klimisch Code: 4 - however considered to be a good quality review of the studies undertaken).

The HSDB reports a KOC of 60 which is estimated with a regression-derived equation based on the log Kow of phenylmercury acetate of 0.71 (Hansch *et al*., 1995; Lyman *et al*., 1990 cf. HSDB). This equation, however, seems inadequate for organomercurials as it only takes into account hydrophobic interactions between sorbent and sorbate and neglects electrostatic interactions of the phenylmercury cation with negatively charged surfaces.

According to a classification scheme applied by Swann *et al*. (1983), the estimated Koc values of 3,164 and 8,333 suggests that phenylmercury acetate is expected to be slightly mobile to immobile in soil. The Koc of 50000 that was determined in sediment, indicate that phenylmercury acetate is immobile in seawater sediments. (Klimisch Code: 2 - reliable with restrictions).

B.4.2.2 Volatilisation

Phenylmercury acetate
Although it can be expected that phenylmercury compounds are predominantly released into air (see chapter B.9.5), the compounds are expected to condensate rapidly on dry matter or water droplets in air due to their low vapour pressure. With dry or wet deposition the compounds enter aquatic and environmental environments.

When used as a plant protection product, a large fraction of the spray residue was found in the soil 30-50 days after application; the rest of the Hg was lost by vaporization (either as the organic compound or after conversion to Hg metal) or by migration to lower soil horizons since water containing organic compound from decomposing vegetable matter can leach adsorbed Hg. (NRCC, 1979 cf. HSDB). (Klimisch Code: 4 - however, HSDB is generally considered to be a reliable database).

Volatilization from moist soil and water surfaces is not expected to be an important fate process because phenylmercury acetate will exist in the dissociated form in the environment. This compound is not expected to volatilize from dry soil surfaces as it is a salt. (SRC Chemfate, 2009). (Klimisch Code: 4 - this conclusion does probably not take the volatility of the subsequently formed inorganic mercury species into account).

Following 28 days of incubation in soil, 14-16 % of applied phenylmercury acetate had volatilised as mercury vapour following biotransformation to inorganic mercury forms. (Kimura and Miller, 1964). (Klimisch Code: 2 - Not guideline study but acceptable quality scientific study).

Volatilization from water surfaces is not expected because this compound is found only in the dissociated form in water (Capel *et al*., 1988). (Klimisch Code: 4 - however considered to be a good quality review of the studies undertaken).

Phenylmercury propionate, octanoate, 2-ethylhexanoate and neodecanoate

No data found. However, as the initial transformation reaction in the environment, dissociation appears to take place quite rapidly in moist soils, it is considered likely that the propionate, octanoate, 2-ethylhexanoate and neodecanoate salts of phenylmercury will not behave much differently from the acetate with regard to volatilization.

B.4.2.3 Distribution modelling

Phenylmercury acetate, propionate, octanoate, 2-ethylhexanoate and neodecanoate
No data found.

A simplified MacKay Level 3 compartmental calculation was performed for phenylmercury acetate using EPI Suite (version 4.0), see Appendix 2. According to the environmental releases listed in Section B.9.5 the emissions were 6.3 to air and 0.3 to waste water. A log Kow of 0.71 and a Koc-value of 8,333 was used for calculation. The following environmental distribution of the substance was estimated:

Air	0.00952%
Water	3.38%
Soil	95%
Sediment	1.64%

B.4.3 Bioaccumulation

B.4.3.1 Aquatic bioaccumulation

Phenylmercury acetate
Different aquatic organisms like fish *Lebistes reticulates*, snail *Helisoma campanulata*, and aquatic plants like pondweed *Elodea canadensis* and rigid hornwort *Ceratophyllum demersum* readily uptake phenylmercury acetate (Fang, 1973). Most of accumulated mercurials were transformed to inorganic mercury and as a minor metabolic product ethylmercuric chloride was found. The biological half-life of mercury containing metabolic products ranged between 43 and 58 days.

MacLeaod and Pessah (1973) investigated accumulation of phenylmercury acetate in muscle tissue of rainbow trout (*Oncorynchus mykiss*) exposed for 4 days at 10ºC. Concentration of mercury in the fish tissue was related to concentration of mercury in the water for phenylmercury acetate. Bioaccumulation factors of 80, 90 and 100 were calculated for aquatic concentrations of 5, 10 and 20 µg Hg/l, respectively.

Rainbow trout fingerlings were fed for 28 weeks with commercial trout feed spiked with phenylmercury actetate (PMA) or ethylmercury phosphate to a Hg concentration of 5 ppm (Matida *et al*., 1971). Fish fed the exposed feed exhibited an apparent decrease in growth and there appeared to be no effect on survivorship. Accumulation in total fish decreased in the following order: methylmercury, ethylmercury, PMA, mercury chloride. The authors state that "mercury in the forms of alkylmercury compounds seems to be easily accumulated in fish bodies, but mercury in the forms of inorganic and aryl compounds does not". The highest concentrations of Hg (given as PMA or ethylmercury) were found in kidney, followed by liver, muscle and residue. Mercury in brain tissue was only detected in fish fed with methylmercury. The authors claim that no organic mercury compounds were found (using a thin layer chromatography method with colorimetric detection) in fish exposed (orally or waterborne) to PMA or mercury chloride. The Klimisch score for this study is considered to be 3 (not reliable based on the lack of proper experimental design, no control organisms and no statistical comparisons).

Biocentration factors for phenylmercury acetate were also estimated using the BCFBAF module in EPI Suite (v. 4.0), see Appendix 2. The model estimates BCFs based on Kow and applies an additional correction factor that accounts for active diffusion of mercury into organisms (Meylan *et al*., 1999). For organic mercury and tin compounds a minimum BCF of 100 is assigned (Meylan *et al*., 1999). For compounds that can be metabolized in biota, a correction factor is applied. The training set used to developed EPI suite BCF model includes 527 chemicals (including two mercury compounds) with experimental and estimated BCF values.

The domain was extracted according to the methodology described in Appendix "Applicability domain". According to the extracted applicability domain phenylmercury acetate was found to belong to the domain of BCF model. For phenylmercury acetate BCFBAF estimates a BCF of 100 both with and without biotransformation taken into account.

Phenylmercury propionate, octanoate, 2-ethylhexanoate and neodecanoate
No experimental data were found.

According to chapter B.4.1.1.1 and outlined by Tang and Nielsen (2010), all five phenylmercury compounds dissociate to more than 90% in water, sediment and soil with a pH between 5 and 9. In this case, one has to focus on the dissociation product instead of the undissociated compound. The mercury containing dissociation product of all five phenylmercury carboxylates is phenylmercury (present predominantly as phenylmercury hydroxide). Also for this compound no experimental data is found. However, if one takes into account that phenylmercury acetate dissociates in the same way as the other four compounds, and that a bioconcentration factor of 100 was experimentally determined for this compound, a bioconcentration factor of 100 can be assumed also for the other four phenylmercury compounds.

One can argue that in environments with a pH between 5 and 6, the percentage of undissociated compound is between 1 and 10%. Because of the higher hydrophobicity of the undissociated compound, the percentage accumulated in biota can be assumed to be considerably higher than the percentage of undissociated compound in water.

BCFs of the undissociated form of the 4 phenylmercury carboxylates were estimated using the BCFBAF module in EPI Suite (v. 4.0), see Appendix 2. In Appendix 2 it was verified that the applicability domain can be extracted to encompass phenylmercury propionate, octanoate, 2-ethylhexanoate and neodecanoate. The module estimating the BCF when metabolism is taken into account was not tested with regard to the applicability domain.

BCFs were also assessed by the BCF baseline model (Dimitrov *et al*., 2005). Only phenylmercury acetate is present in the training set of the model but it is out of the model domain because the uptake of metals could be based not only on passive diffusion. The model predicts the maximum potential for bioconcentration and biocencentration corrected accounting for mitigating factors such as metabolism, molecular size, and water solubility.

Estimated BCFs for the dissociated and undissocited forms of the phenylmercury are listed inTable B-6.

Table B-6 BCFs for dissociated and undissociated compounds. Predicted BCFs for undissociated compounds according to the BCF baseline model (Dimitrov *et al*., 2005) and by the BCFBAF module in EpiSuite 4.0. Maximum potential for bioconcentration (BCFmax) and bioconcentration corrected accounting for mitigating factors (BCFcorr). All BCF values are in L/kg wet weight

Chem. Name	**BCF for dissociated compound**	**BCF for undissociated compound**		
		BCF baseline model		**EpiSuite 4.0**
		BCF max	**BCF corr**	**BCF max (without metabolism)**
Phenylmercury acetate	100	14	7.3	100
Phenylmercury propionate	100	20	12	100
Phenylmercury 2-ethylhexanoate	100	650	350	3546

Phenylmercury octanoate	100	740	283	3965
Phenylmercury acetate neodecanoate	100	3200	1300	14890

The estimated BCF are between 7.3 and 14,890 for the phenylmercury compounds. Maximum BCFs calculated with the BCF baseline model probably underestimate the bioaccumulation potential of phenylmercury compounds because active transport of the compounds through the cell membrane that is based on interaction with cell proteins, is not taken into account. The BCFBAF module in EpiSuite takes into account active transport of mercury compounds through the cell membrane and calculates therefore considerably higher values.

Metabolism of the phenylmercury compounds can be expected in organisms, however, since the metabolic products will also be hazardous substances (e.g. inorganic mercury or other organomercuric metabolites) maximum BCFs from EpiSuite are used in the estimation of the BCF. They represent a worst case scenario for the bioaccumulation potential of the undissociated species of the phenylmercury compounds.

Based on the BCF values for dissociated compounds and undissociated compounds, the BCF for water with a certain pH can be calculated. If water with a pH of 5 is assumed, ca. 90% of a phenylmercury compound is dissocitated and 10% is undissociated. The BCF for this water can be calculated as follows:

Estimated BCFs for the 5 phenylmercury compounds in water with pH 5 are listed in Table B-7. BCFs at higher pHs are expected to decrease and converge to BCFs for dissociated species. These estimated BCFs between 100 and 1,579 will be used for the PBT assessment.

$$BCF = Portion_{dissociated\ species} * BCF_{dissociated} + Portion_{undissociated\ species} * BCF_{undissociated}$$

Table B-7 Estimated BCFs for the 5 phenylmercury compounds in water with pH 5

CAS #	Chem. Name	BCF in water with pH 5
62-38-4	Phenylmercury acetate	100
103-27-5	Phenylmercury propionate	100
13302-00-6	Phenylmercury 2-ethylhexanoate	445
13864-38-5	Phenylmercury octanoate	487
26545-49-3	Phenylmercury acetate neodecanoate	1 579

Other mercury compounds

Methylmercury

The inorganic mercury species eventually formed by biotransformation reactions (as described in Section B.4.1.2) can, under anaerobic conditions, undergo bacterially mediated

methylation to methylmercury. Thereby, the release of all the above substances also implies a risk of formation of methylmercury, which is known to bioaccumulate strongly in aquatic food webs via the diet and can be up to 10^7 times higher than the concentration measured in the water (Weiner *et al*., 2003).

Fish appears to strongly accumulate methylmercury. Nearly 100 percent of mercury that bioaccumulates in predator fish is methylmercury. Most of the methylmercury in fish tissue is covalently bound to protein sulfhydryl groups. This strong binding is the reason for a long half-life of about two years in biota (Wiener and Spry, 1996 as cited in UNEP, 2002). As a consequence, a selective enrichment of methylmercury (relative to inorganic mercury) can be observed as one moves from one trophic level to the next higher trophic level. In contrast to other mercury compounds the elimination of methylmercury from fish is very slow (US EPA, 1997 as cited in UNEP, 2002).

Given steady environmental concentrations of methylmercury, tissue concentrations of a given fish species tend to increase with increasing age as a result of the slow elimination of methylmercury and continous uptake of methylmercury with food. This process is intensified because the amount of food increases with increasing age and also the type of food changes towards organisms of a higher trophic level when fish get older. Therefore, older fish typically have higher mercury concentrations in the tissues than younger fish of the same species (UNEP, 2002).

The high bioaccumulation potential of methylmercury is also reflected in the substance data sheet for mercury for the Water Framework Directive where BCFs of 8,140 (geometric mean for fish) up to 85,700 are reported for rainbow trout (*Oncorhynchus mykiss*). Hill *et al*. (1996) showed that the bioconcentration factors for methylmercury increased between 0.5-1.5 log units in lower trophic levels of a freshwater ecosystem. Furthermore, the substance data sheet for mercury presents bioaccumulation factors (BAF) for methylmercury in water and biota in the field. The BAF values vary up to four orders of magnitude - from a geometric mean of 21,700 up to 79,000,000 for sharks as top predators in the marine environment. In the document it is stressed that within one trophic level BAFs generally vary up to two orders of magnitude due to various site specific biotic and abiotic factors. The Scientific Committee on Health and Environmental Risks (SCHER) reported in its opinion on the environmental risks and indirect health effects of mercury in dental amalgam (SCHER 2008) that BAFs for fish species measured in the field differ from about 20,000 to over 20,000,000.

Field observations are mentioned in literature that report intoxications and reproductive impairment in certain avian species (divers, sea eagle, fish eagle) eating fish contaminated with methylmercury at concentrations between 0.2 and 0.7 mg/kg (Euro Chlor, 1999).

The mentioned reports and publications clearly show that methylmercury is biomagnified significantly through the food web with negative impact on top predators.

In contrast, inorganic mercury is not transferred via the food web and does not biomagnify.

Diphenylmercury

Diphenylmercury is easily taken up by organisms due to its moderately high lipophilicity. According to Brinckman & Bellama (1978) diphenylmercury interacts weakly with donor molecules and does not form stable complexes. Diphenylmercury is more rapidly excreted by rats than phenylmercury and metallic mercury and even if accumulation is initially higher in

the brain and fatty tissues of rats, concentrations rapidly drop due to metabolism to inorganic mercury (Brinckman & Bellama, 1978).

B.4.3.2 Terrestrial bioaccumulation

Phenylmercury acetate, propionate, octanoate, 2-ethylhexanoate and neodecanoate
No experimental data on terrestrial bioaccumulation of phenylmercury acetate, propionate, octanoate, 2-ethylhexanoate and neodecanoate was found.

However, if bioaccumulation in terrestrial organisms is assumed to be similar between aquatic and terrestrial organisms, biota-soil-accumulation factors (BSAFs) can be calculated based on aquatic data and applying a Koc of 8,333 L/kg and assuming an organic carbon content of 2% in soil.

BSAFs for dissociated and undissociated species are presented in Table B-8

Table B-8 BSAFs estimated based on aquatic bioconcentration factors

CAS #	Chem. Name	BSAF for dissociated compound	BSAF for undissociated compound (assuming metabolism)
62-38-4	Phenylmercury acetate	0.6	0.6
103-27-5	Phenylmercury propionate	0.6	0.6
13302-00-6	Phenylmercury 2-ethylhexanoate	0.6	21.3
13864-38-5	Phenylmercury octanoate	0.6	23.8
26545-49-3	Phenylmercury neodecanoate	0.6	89.3

If a soil with pH 5 is assumed, the 90% of the phenylmercury compounds are dissociated and 10% are undissociated. The BSAF for this soil can be calculated as follows:

$$BSAF = Portion_{dissociated\ species} * BSAF_{dissociated} + Portion_{undissociated\ species} * BSAF_{undissociated}$$

Estimated BSAFs for the 5 phenylmercury compounds in soil with pH5 are listed in Table B-9. BSAFs in soils with higher pHs are expected to decrease and converge to BSAFs for dissociated species.

Table B-9 BSAF in soil with pH5

CAS #	Chem. Name	BCF in water with pH 5
62-38-4	Phenylmercury acetate	0.6
103-27-5	Phenylmercury propionate	0.6
13302-00-6	Phenylmercury (2-ethylhexanoate)	2.7
13864-38-5	Phenylmercury octanoate	2.9
26545-49-3	Phenylmercury neodecanoate	9.5

B.4.3.3 Summary and discussion of bioaccumulation

In environments with a pH 5 – 9, all five phenylmercury substances are mainly dissociated to the common intermediate phenylmercury and the corresponding carboxylate. The phenylmercury (predominantly present as hydroxide at pH 5 - 9) has a small bioaccumulation potential with BCFs of about 100. For the undissociated compound, estimated BCFs differ between different models. Based on the EpiSuite model bioconcentration factors are estimated to 100 for phenylmercury acetate and propionate but are significantly higher for the other three compounds, representing a worst case scenario for the bioaccumulation potential of the undissociated species of the phenylmercury compounds. Taking into account the dissociation, estimated BCFs for the 5 phenylmercury compounds in water at pH 5 are estimated to be between 100 and 1,579.

In the terrestrial environment BSAFs are based on aquatic BCFs and vary between 0.6 and 9.5 for the phenylmercury compounds.

Phenylmercury compounds are expected to be degraded to inorganic mercury species. These can be transformed to methylmercury in oxygen deficient environments. BCFs for methylmercury in fish of 8,140 up to 85,700 are reported demonstrating that methylmercury is known to bioaccumulate to a large extent in higher organisms such as mammals, birds and fish. BAF measured in the field for fish species range from about 20,000 to over 20,000,000, substantiating that methylmercury is biomagnified significantly through the food web.

B.4.4 Secondary poisoning

Phenylmercury acetate, propionate, octanoate, 2-ethylhexanoate and neodecanoate
No data found.

However, referring to Section B.4.3 it can be assumed that releases of phenylmercury compounds will contribute to the formation of inorganic mercury, which in turn can be transformed into methylmercury under (primarily) anaerobic conditions. This substance is

known to bioaccumulate and result in secondary poisoning, of which the most notable case is the Minamata disease case in Japan in the 1950'ies.

B.5 Human health hazard assessment

The assessment of the human health hazards of the five phenylmercury compounds and their metabolites, degradation products and transformation products is based on studies available in the open literature. Relatively few studies were found for phenylmercury acetate (PMA) and the available studies did not cover all the hazard classes listed in the CSR template (REACH annex I) as demanded in REACH annex XV for restriction proposals. The available studies are often old, they are incompletely described and/or they were not performed according to any guideline or GLPs. Major deviations from a relevant guideline are shown as "comments" in the study summaries.

In the text which follows, the most relevant literature for PMA has been reported and evaluated. In most cases original study reports have been assessed, otherwise this is stated. No studies were found for phenylmercury octanoate, phenylmercury neodecanoate and phenylmercury 2-ethylhexanoate and only one study was found for phenylmercury propionate. Hence, an assessment of these compounds could not be performed. The database for all these compounds was very limited or non-existing. Applying the OECD (Q)SAR Application Toolbox gave no further information on health effects.

There is support from information on degradation assessed theoretically for the environment that the 5 phenylmercury substances are degraded in a similar way and rate (see Section B.4). Such information is lacking for the health part (see Section B.5.1). There is too little information to assume that the 5 phenylmercury substances will have similar toxicokinetics in humans and other mammals. Therefore, read-across based on health effects has not been done.

The 5 phenylmercury substances are degraded in the environment. Humans are exposed via the environment, and the toxicology of the relevant breakdown products are described under each effect in Section B.5. For the metabolites, degradation products and transformation products there are large amounts of data in the open literature. The assessment of these compounds is therefore based on review reports, mainly on human data.

B.5.1 Toxicokinetics (absorption, metabolism, distribution and elimination)

B.5.1.1 Non-human information

Phenylmercury acetate

"Distribution of mercury in rats following oral and intravenous administration of mercuric acetate and phenylmercuric acetate" (Prickett et al., 1950)

Materials and methods: An aqueous solution of PMA was administrated to three to four young adult male rats (bw 250-300g, strain not reported) intravenously (by femoral vein) or by gavage under light ether anaesthesia. The rats were administrated a single dose of mercury given as PMA. The dose was from 10 to 120µg mercury/animal. PMA was dissolved in 0.25ml and 2ml volume for the intravenous injection (iv) and oral administration,

respectively. The animals were sacrificed at intervals of 2, 6, 24, 48 and 96 hours after treatment. Tissue, blood and excreta were analysed for mercury. Faeces and urine were collected separately and the contents of the urine bladder, cecum and large intestine were included in the corresponding sample.
Comment: The quality of the study is acceptable.
Results: Following iv and oral administration, the concentration of mercury was higher in kidney compared with liver 24 hours after administration. The storage of PMA was mainly in the kidney, but also to some extent in the liver. Tissues such as spleen, muscle, bone and brain were found to contain minor levels of mercury after iv administration of PMA. The concentration of mercury in the kidney and liver after iv administration of the highest dose of PMA decreased slowly from 24 hours after administration to the end of the experiment.
For both administration routs the highest level of mercury was found in faeces. Twenty four hours after iv administration of 120µg mercury as PMA, approximately 40µg mercury was found in the faeces, while only 4µg mercury was found in the urine in a total (Table B-10).

Table B-10 Comparative tissue distribution of mercury following oral and intravenous administration of 120µg mercury as PMA

Hours		Kidney (µg/g)	Liver (µg/g)	Blood (µg/g)	Urine total (µg)	Faeces total (µg)
2	(iv) (O)	4.2 5.3	1.8 1.2	1.9 0.33	0.43 0.64	1.7 9.0
6	(iv) (O)	11 7.1	1.1 1.1	1.8 0.52	0.74 2.7	9.3 24
12	(iv) (O)	14 10	0.85 0.81	1.9 0.46	1.4 2.3	19 37
24	(iv) (O)	16 7.9	0.78 0.74		3.9 2.8	37 45
48	(iv) (O)	14 9.5	0.48 0.58		3.9 5.3	40 78

(iv) Intravenous, (O) oral. Each value represents average of 3 animals.

"Distribution of phenylmercuric acetate in rat" (Niwaguchi and Otsuka, 1966)
Materials and methods: 203Hg-labelled PMA suspended in arabic gum (5 mg/kg, specific activity of approximately 2 µc/mg Hg) was given Wister-strain rats (bw 200-300g). One ml of the solution was administrated once gavage by a stomach tube. Rats were killed by bleeding 24, 48 and 96 hours after the exposure. The radioactivity was determined in organs and tissues by scintillation counter. Intracellular localization of 203Hg in liver and kidney homogenates was studied in different fractions after centrifugation.

Comment: The OECD test guideline 417 recommends at least two dose levels when a single dose administration is used. In this study only one dose level is used. The number of animals and sex is unknown.

Results: Little 203Hg were distributed to the brain, heart and spleen at 24 and 48 hour after administration (Table B-11). After 3 days the level of 203Hg was not detectable in the heart and brain. The highest levels of 203Hg were found in the kidney and liver and the levels were not decrease markedly after three days.
For the intracellular localization, most of the 203Hg was found in the supernatant (55-70%) and in the 900 x g fraction (27-35%) in both liver and kidney cells (Table B-12). The 900 x g fraction includes unbroken cells, blood-corpuscles and connective tissue besides nuclei. In addition low levels of 203Hg was found in the nuclei (Table B-13). Thus, in cells from liver

and kidney the 203Hg was mainly bounded to soluble proteins in the intracellular fluid and little was taken up by the nuclei.

Table B-11 Percentage of 203Hg found in tissues after oral administration of 5 mg/kg bw 203Hg-PMA

Tissue	24 h (%)	48 h (%)	96 h (%)
Kidney	9.8	9.7	8.0
Liver	3.0	1.5	1.5
Blood	2.1	0.3	0.1
Spleen	0.09	0.06	0.01
Heart	0.03	0.03	0.0
Brain	0.008	0.002	0.0
Intestines	9.8	1.3	0.4
Stomach	1.2	1.0	0.1
Total	26	13.9	10.1

Table B-12 Intracellular percentage of 203Hg in liver and kidney cells.

	24 hours		48 hours		96 hours	
	Liver (%)	Kidney (%)	Liver (%)	Kidney (%)	Liver (%)	Kidney (%)
Fraction						
900 x g	30.9	28.9	28.5	35.1	27.2	35.0
10^4 x g	5.1	4.7	7.5	5.0	8.8	0.0
10^4 x g	5.9	6.5	5.4	3.6	7.8	0.0
Sup.	58.1	60.0	58.7	56.4	55.2	65.0

Table B-13 203Hg in nuclei from liver and kidney cells

Tissue	24 hours	48 hours	96 hours
Liver	1.8	0.07	0.0
Kidney	2.4	0.1	0.0

"Distribution and excretion of methyl and phenyl mercury salts" (Gage, 1964)

Materials and Methods: Female albino Wistar rats (bw125-135g) were injected subcutaneously three times a week for up to six weeks with an aqueous solution of PMA. The dose was equivalent to 0.15 mg mercury/rat (0.45mg mercury/week) and there were six rats in each group. At the end of the six week period the body weight range for treated animals was from 170 to 190g.

Groups of five to six rats were placed in metabolism cages provided with a separator for urine and faeces for one week. The excreta were collected and then the animals were killed. Liver, kidneys, brain and spinal cord, spleen, and area of shaved skin from the injection site were analysed for organic and total mercury content. This procedure was repeated weekly throughout the six weeks of the experiment. A more complete tissue analysis was made from the finale group.

In addition, one group of five female albino Wistar rats received a single subcutaneous dose of PMA equivalent to 0.5 mg mercury/rat. The excreta were collected and analysed over a period of three weeks.

Comment: The weight of the rats was low and may indicate young animals, but their age was not reported.

Results: The organic and total mercury content in tissues and excreta, shown in Table B-14and Table B-15, gives an indication of the distribution, accumulation and excretion of mercury during the six week experiment.

PMA was readily absorbed from the injection site, and the low blood concentration indicated that it was rapidly removed by the tissues (Table B-14). High content of mercury was found in the skeletal muscle where metabolism may occur, and in the hair. Most of the PMA was removed from the plasma by the liver and kidneys where it was rapidly metabolised and excreted with only a proportion appearing unchanged in faeces and urine. Most of the PMA was excreted via faeces.
No toxic effects were observed after treatment with the equivalent of 0.45 mg mercury as PMA per rat per week for six weeks. No measurable accumulation of mercury was found in the central nervous system.

Table B-14 Organic and total mercury tissue content in rats dosed with the equivalent of 0.45 mg mercury per week

	PMA						
Time (week)	**1**	**2**	**3**	**4**	**5**	**6**	
Kidney: organic total	 3 96	 1,5 93	 2 110	 1 91	 1 117	 3 117	(µg/g) 2 90
Liver: organic total	 <2,5 15	 <2,5 10	 <2,5 20	 <2,5 12	 2 20	 <1 8	 <0.2 1.3
Brain and cord: organic total	 <1 <2	 <1 <2	 <1 <2	 <1 <2	 <1 <2	 <1 <2	 <0.5 <1
Spleen: organic total	 <0.4 <0.6	 <0.4 <0.6	 <0.5 <1	 <0.5 <0.8	 <0.8 <1.5	 <0.6 <1	 <0.5 <1
Skin (injection site): organic total	 10 18	 11 25	 13 36	 7 15	 1.5 1.5	 2.5 12	 0.4 2
Muscle: organic total						 103 232	 1.3 3
Red cells: organic total						 4 6	 0.7 1
Blood plasma: organic total						 1 1	 0.2 0.2
Intestine: organic total						 <5 <10	 <0.5 <1
Heart muscle: organic total						 <0.3 <0.6	 <0.5 <1
Hair: organic total							 28 14
Body fat:							<5

Figures are in µg mercury per rat and are the average of five to six rats taken at weekly intervals. The second column of the last group shows the calculation in µg/g tissue. The content of blood and muscle is estimated from the assumptions that each rat contained 10 ml blood and that the skeletal muscle constituted 43% of the body weight.

The day after given a single dose of PMA to the rats, all the recovered mercury in the urine was organic. The level of organic mercury in the urine diminished rapidly to very low values (Table B-15). Inorganic mercury appeared in the urine on the second day and increased to a maximum by the fourth day and then decreased until the end of the second week. These observations suggest that circulating PMA enters the kidneys and is in part rapidly excreted unchanged in the urine and in part converted to inorganic mercury which is not as readily

available for excretion. Most of the excretion was via faeces. After given a single dose most of the mercury in faeces was inorganic and it reached a maximum at day 3 to 4. During the third week after given a single dose, only a small amount (< 8 µg) of mercury was excreted. About two-thirds of the dose administrated was recovered in the excreta.

Table B-15 Weekly organic and total mercury excretion by rats dosed with the equivalent of 0.45 mg mercury per week for six weeks

	PMA					
Time (week)	**1**	**2**	**3**	**4**	**5**	**6**
Urine: organic total	 7 44	 16 89	 10 85	 25 99	 13 106	 7 102
Faeces: organic total	 <18 159	 <17 185	 21 182	 20 116	 <12 185	 <10 148
Total in excreta:	203	274	267	215	291	250

Figures are in µg mercury/ rat / week and are the average of five to six rats.

Table B-16 Excretion of organic and total mercury after a single subcutaneous dose equivalent to 1 mg mercury

	PMA			
	Urine		**Faeces**	
Time	Organic	Total	Organic	Total
First week: Day 1	22	22	1.8	17
2	2.6	6	3.2	106
3	0.8	16	5	229
4	<0.4	23	<3	
5	<0.2	10.5	<1.5	54
6	2.1	10	<3	38
7	0.3	10.5	<4	43
Second week	4	26	5	75
Third week		<3		<5
Total		124		552

Figures are in µg mercury/ rat and show the average of five rats.

"Distribution and excretion of mercury compounds after single injection" (Swennsson et al., 1959)

Materials and methods: Three experiments were performed and reported in this paper. Experiments I: Rats were anesthetized by an intraperitoneal injection of tribromoethanol and exposed to PMA through the femoral vein. The dose was given as a single injection and was 100 µg mercury/kg bw, corresponding to 167.9 µg PMA/kg bw which was approximately 1% of the LD50 value. Ten rats were killed with ether after 3 hours and 1, 4, 16, and 32 days after exposure. The mercury content in the organs was estimated.

Experiment II: Two dogs were used to study the mercury content in blood and urine immediately after an intravenous single injection in the saphenous vein with PMA (0.1 mg mercury/kg bw). Blood was sampled from the inferior vena cava and urine was collected from the bladder by a catheter for 0-240 minutes after injection.

Experiment III: Human blood cells were exposed to 1-10 ppm mercury given as PMA to study the distribution of PMA in blood. The PMA was added to citrated blood in vitro, and the mercury content of whole blood and plasma was determined.

The radiochemical analysis involved counting of β-particles with a Geiger end-tube on a thin precipitate of mercuric sulphide.

Comment: The OECD test guideline 417 recommends at least two dose levels when one single dose administration is used. In this study only one dose was used.

Results: In the experiment with rats (experiment I), the highest concentration of mercury was found in the kidney. After 24 hours 25µg/g (wet-weight tissue) was found in the kidney. Between 4 to 16 days after exposure, 5-6 µg/g was found and after 32 days the level was reduced to 0.1 µg/g (Table B-17).

Table B-17 Mercury content in different organs of the rat*

Time after injection	Kidney	Liver	Brain	Blood
3 hours	0.2	0.072	0.070	0.900
24 hours	25	0.700	0.030	0.740
4 days	6.6	0.120	0.030	0.210
16 days	5.2	0.110	0.030	0.010
32 days	0.1	0.130	0.0005	0.020

*Mercury content is given in µg Hg/g wet-weight tissue. The dose injected was 100 µg Hg/kg bw. Each figure is the mean of 10 animals.

The relationship between the mercury content in blood and the excretions in urine was studied in dogs (experiment II). It was observed that the excretion of PMA in urine started immediately after the injection and that it diminishes nearly parallel to the mercury concentration in the blood. During the first four hours, 4% of the PMA was excreted in urine. The highest level of mercury was found in the kidney four hours after exposure. In both rats and dogs no tendency for mercury to accumulate in the brain was observed.

Table B-18 Mercury content in different organs in dogs four hours after intravenous injection*

Organ	µg Hg/g tissue
Liver	0.40
Kidney	3.55
Brain	0.015
Cerebellum	0.073
Colon	0.42

*Mercury content is given in µg Hg/g wet-weight tissue. The dose injected was 100 µg Hg/kg bw. Each figure is the mean of 10 animals.
The dose injected was 100 µg Hg/kg bw. Each figure is the average of two animals.

In the in vitro studies (experiment III) the ratio between the mercury content of plasma and whole blood was 0.1 for the organic compounds and 0.8 for the inorganic compounds. This indicates that organic mercury compounds were chiefly bound to the erythrocytes in the blood, whereas the inorganic compounds were bound to the plasma.

"Renal uptake, excretion, and retention of mercury" (Berlin, 1962)
Materials and methods: Groups of male rabbits (bw 3-4 kg) were administrated 203Hg labelled PMA by intravenous infusion into the jugular vein. The total infused dose of PMA contained approximately 8 mg mercury, which gave a blood concentration of about 10 µg Hg/ml blood. The method enabled measurement of renal extraction from the blood, urinary excretion and blood concentration of radioactive mercury. Arterial blood concentration, the urinary excretion of mercury as well as the creatinine clearance were measured for periods of 2 to 3 hours. At the end of the experiment the content of radioactive labelled mercury was measured in the kidney. The mercury concentration was measured by a scintillation detector.

Comments: There was no record of the number of animals in the groups.

Results: Following infusion of PMA a rapid increased mercury concentration in blood as well as a similar increase in the urine was observed. This could be interpreted as a positive correlation between urinary excretion and blood concentration. This relation was further elucidated by rapidly increasing the blood concentration by rapid injections of PMA. The results support the previous observations that there is a strong correlation between the levels of mercury in the blood and urine. In the present experiment no tendency for cumulative excretion was observed.

High accumulation of mercury was found in the kidneys. The excretion of mercury in the urine was only a fraction of the total amount accumulated in the kidneys during the experiments.

The distribution of mercury in the blood was examined. About 10% of the mercury in the blood was found in the plasma. Most of the mercury in the blood was bound to the red blood cells.

Table B-19 The distribution of mercury between blood corpuscles and plasma at the end of 4 experiments

Experiment	% Hg in RBC	% Hg in Plasma
1	96.6	9.4
2	93.4	6.6
3	84.2	15.8
4	90.7	9.3

"The absorption of phenylmercuric acetate from the vaginal tract of the rat" (Laug and Kunze, 1948).

Materials and methods: Young female rats (average 250 g) were light anesthetized and were administrated 9, 18 or 36 µg mercury in a PMA solution via a small cotton pledged inserted into the vagina. PMA has previously been used in contraceptive for humans. The lowest dose in these experiments was estimated to be 50 % larger than the average human dose when the substance was used as a spermaticide. Exposure time was 24 hours and the rats were in this period placed in leather holders to the bottom of the cage. After exposure the vaginas were washed. Four animals were killed 0, 24, 48 or 168 hours after exposure. The blood supply to the vaginal mucosa is closely controlled by the oestrus cycle of the animal and is enhanced during oestrus. Thus, examination of absorption of PMA solution during oestrus compared to anoestrus period was performed. The results indicated no difference in absorption.

Comments: Exposure via the vagina is not a standard exposure route according to guideline, but relevant for examining possible effects by using PMA as a spermicide. There is no information concerning the rat strain. The body weight is given as an average, but without the range.

Results: Exposure to doses from 18 µg mercury in a PMA solution caused moderate to severe irritation to the vaginal mucosa. After 24 hours, between 24-31 % of the applied dose (9-36 µg mercury) was measured in the liver and the kidney as a total. The highest mercury level was found in the kidney. Elimination from this organ was slow compared to elimination via liver. 168 hours post administration of 18 µg mercury intravaginally the levels in the kidneys were only decreased by 12 %, while all the mercury was eliminated from the liver. Also a larger amount of mercury was found in the kidney compared to liver at all time points. The

results indicate that the distribution of mercury to the kidneys is significant and that the elimination of mercury from the kidney is relatively slow.

Table B-20 Reduction of mercury in liver and kidney with time

18 µg mercury injected					36 µg mercury injected				
Hours after end of exposure	Liver* µg Hg	Kidney* µg Hg	Total µg Hg	Per cent of injected dose	Hours after end of exposure	Liver* µg Hg	Kidney* µg Hg	Total µg Hg	Per cent of injected dose
0	1.9	2,4	4,3	24	0	3,7	5,6	9,3	26
24	1,7	2,6	4,3	24	24	1,8	4	5,8	16
48	0,83	2,7	3,5	19	48	1,6	5,7	7,3	20
168	0	2,1	2,1	12	168	0,98	3,6	4,6	13

*Average of 4 rats on each dose and at each period. Mercury was given in PMA solution.

"Absorption, distribution and excretion of phenylmercuric acetate" (Miller, 1960)
Materials and methods: Chicks (bw 400-1200g), rats (Sprague-Dawley) and dogs (young, healthy, stray dogs), bw for rats and dogs not reported, were exposed to PMA. Recrystallized PMA was dissolved in isotonic phosphate buffer (finale pH of 7.2) and was used for intramuscular or intravenous injections. For the oral administration (given in the feed) PMA was used without buffer. The dose of PMA given intramuscular or intravenous corresponded to 3.0 mg Hg/kg bw, while for the oral study the doses corresponded to 7.5 and 30 mg Hg/kg bw. Groups of animals were killed 1, 3, 12, 24, 48, 72 and 96 hours after exposure. Tissues, blood, urine and faeces were removed/collected and analysed.

Comment: There is a lack of information concerning the animal weight, age and sex. Clinical symptoms are not reported. The number of animals per group is also provided incompletely.

Results:
Chicks: Fifty birds were injected with 3.0 mg/kg bw in the breast muscle. Almost all the mercury in the liver up to 3 hours after injection was in the form of PMA (Table B-21). One hour after injection approximately half of the total mercury level in the kidneys was PMA. This indicated that metabolism of PMA already had taken place in the kidneys. By 48 hours the amount of PMA in the organs approached the limit of detection. The total mercury in the liver remained fairly constant up to 96 hours, while the mercury level in the kidney increased.

Table B-21 PMA and mercury in the organs of chicks after intramuscular injection of 3.0 mg mercury as PMA per kg bw

Hours after injection	Average ppm PMA		Average ppm mercury	
	Liver	Kidney	Liver	Kidney
1	16	9	18	15
3	14	7	18	18
12	6	8	13	28
24	4	5	18	39
48	3	3	22	44
72	2	3	15	37
96	1	2	13	40

Doses of 7.5 or 30 mg mercury (given as PMA) per kg bw were administrated orally to 43 birds (Table B-22, Table B-23). At the lower dose level, the PMA present in the liver accounted for all the mercury during the first hour (Table B-22). The levels of PMA decreased with increasing time after exposure. Analyses of the blood indicated that almost all mercury in the blood was in the form of PMA (Table B-22, Table B-23). The total mercury levels in liver and kidney was similar to that following intramuscular injection. The highest

dose of PMA given in the feed resulted in higher concentrations in the tissues and blood compared with lower doses (Table B-23). The pattern of distribution was quite similar comparing oral and intramuscular injection administration routs in chicks.

Table B-22 PMA and mercury in chick tissue after oral dose of PMA

Hours after dosage	7.5 mg Hg as PMA/kg bw					
	Average ppm PMA			Average ppm mercury		
	Liver	Kidney	Blood	Liver	Kidney	Blood
1	8	8	2	8	14	2
3	13	14	5	20	37	7
12	9	8	6	34	64	6
24	3	3	6	40	61	7
48	3	3	2	27	55	3

Table B-23 PMA and mercury in chick tissue after oral dose of PMA

Hours after dosage	30.0 mg Hg as PMA/kg bw					
	Average ppm PMA			Average ppm mercury		
	Liver	Kidney	Blood	Liver	Kidney	Blood
1	-	-	-	-	-	-
3	40	40	25	59	86	25
12	22	24	21	101	144	25
24	12	14	20	104	107	25
48	6	6	8	126	112	17
72	4	3	4	72	72	5

Chicks were given feed containing PMA in varying lengths of time (Table B-24). Some of the birds were then given commercial diet without PMA for 24 or 48 hours. Appreciable amounts of PMA were found in the organs of the birds that had eaten feed containing PMA. However, after 24 hours on a commercial diet, the amount of PMA had been decreased to a barely detectable level. The amount of the total mercury was larger compared with the amount of PMA which indicate that PMA has been metabolised to other mercury compounds.

Table B-24 PMA and mercury in chick organs after feeding a ration containing PMA

PMA		PMA in ration (ppm)	Average PMA		Average mercury	
On (hr)	Off (hr)		Liver (ppm)	Kidney (ppm)	Liver (ppm)	Kidney (ppm)
24	0	600	14	10	65	106
48	0	600	12	13	94	171
72	0	600	10	16	79	146
24	24	600	4	5	59	111
48	24	600	3	3	62	168
48	48	600	3	3	34	70

Rats: Twelve rats were housed in metabolism cages and injected intramuscularly with 3 mg mercury as PMA/kg bw (Table B-25). Highest level of PMA and mercury were found in the kidney, while only minute amounts were measured in the brain. Slightly less than half of the total mercury excreted in the urine was in the form of PMA. Faecal excretion of mercury increased rapidly with time.

Table B-25 PMA and mercury in rat tissue after intramuscular injection of 3 mg mercury as PMA per kg bw.

Hours after injection	3 mg Hg as PMA/kg bw									
	Average ppm PMA					Average ppm mercury				
	Liver	Kidney	Spleen	Brain	Urine	Liver	Kidney	Brain	Urine	Faeces
12	6	21	6	1	1.6	8	80	0	3.6	1
24	5	10	6	0	1.9	12	76	0	4.5	25
48	3	9	2	1	0.8	13	93	1	2.1	79

Dogs: Four dogs housed in metabolism cages and injected intravenously with 3 mg mercury as PMA/kg bw (Table B-26). A large amount of the PMA was accumulated in the spleen as PMA. Urinary excretion of PMA was proportionally less for dogs compared with rats.

Table B-26 PMA and mercury in dog tissue after intravenously injection of 3 mg mercury as PMA per kg bw.

Weight of dog (kg)	Sex	Hours after injection	3 mg Hg as PMA/kg bw											
			Average ppm PMA						Average ppm mercury					
			Liver	Kidney	Spleen	Blood	Brain	Urine	Liver	Kidney	Spleen	Blood	Brain	Urine
7.0	F	1	23	25	103	16	0	0.3	44	45	111	30	2	2
11.5	F	3	6	32	84	-	1	0.8	15	97	94	-	0	7
10.9	M	12	16	22	58	10	2	0.4	34	81	64	12	1	12
6.4	M	24	14	9	5	5	0	0.3	30	101	14	-	0	10

These studies indicate that PMA is absorbed unchanged regardless of administration route. Transportation via blood appears to be in the form of PMA. Limited data from the dog study indicates that a great proportion accumulates as PMA in the spleen in dogs. In the liver and kidneys the PMA appears to be metabolised into inorganic mercury and accumulated. The metabolism was fairly rapid. Detectable amounts of PMA occurred for approximately 96 hours. The results indicate that rats excrete a greater proportion of PMA via urine compared with dogs. Most of the mercury was excreted via faeces.

Phenylmercury propionate
No data found.

Phenylmercury octanoate
No data found.

Phenylmercury neodecanoate
No data found.

Phenylmercury 2-ethylhexanoate
No data found.

B.5.1.2 Human information

Phenylmercury acetate

"Phenylmercuric Acetate as a contraceptive" (Nicholson et al., 1944)
The absorption of PMA from the vagina was studied in six women. A catheter was inserted in the bladder and a 24 hour specimen of urine was collected from each patient for mercury analysis as a control. Then jelly with 0.05% PMA (1.788 mg mercury) was inserted in the vagina and a second 24 hour urine specimen was collected and analyzed for mercury. In the control samples the total average level of mercury was 22 μg, while after using the jelly with PMA the average level was 83 μg. It was estimated that 3.4% of the inserted mercury was excreted. To examine exposure to repeated instillations 14 women who had used the jelly for six months or more were included in the study. A 24 hour specimen of urine was collected from each patient for mercury analysis. The total average level for this group was 76 μg. The

total average mercury levels in the 24 hours urine specimen was almost identical. No evidence of vaginal irritation or other toxic effects were observed.

Phenylmercury propionate
No data found.

Phenylmercury octanoate
No data found.

Phenylmercury neodecanoate
No data found.

Phenylmercury 2-ethylhexanoate
No data found.

B.5.1.3 Summary and discussion on toxicokinetics

Phenylmercury acetate
Low blood concentration after administration of PMA orally or via injection indicates that PMA is rapidly removed by the tissues. In an in vitro study it was found that most of the PMA in human blood was bound to erythrocytes, while inorganic mercury compounds were bound to plasma. Most of the mercury in the blood was in the PMA form. In all species that were examined, PMA was found to be taken up and stored in kidney and liver. In mammals the highest levels were measured in kidneys. In these tissues PMA was mainly bound to the soluble proteins in the intercellular fluid and little was taken up by the nuclei. Only minor levels have been found in brain, heart, bone, CNS and spleen. In one study high content of mercury was found in hair and skeletal muscles (rats) and in dogs high levels of PMA were found in the spleen.

The results indicate that the excretion of PMA begins immediately after injection and diminishes nearly parallel with the concentration in blood. In all tissues, except for kidney and liver, the mercury level was markedly decreased after 96 hours post oral administration. The mercury levels in kidney and liver were at a maximum level approximately 24 hours after injection. PMA accumulated in kidney and liver. The mercury levels in liver decreased faster compared to the levels in kidney.

Short time after injection most of the PMA was recovered as organic mercury in the urine, but the level diminished rapidly. Recovered levels of inorganic mercury increased with time to a maximum at day four after a single injection. The results indicate that PMA enters the kidney and is in part rapidly excreted unchanged in the urine and in part metabolised to inorganic mercury compounds which are not as readily available for excretion. The metabolism is fairly rapid. Only a small proportion of the PMA appeared unchanged in the faeces and urine. For both oral and intravenous administration routs, the highest level of mercury was excreted via faeces. For dogs urinary excretion was found to be lower than for rats. Faecal excretion increased rapidly with time and two days after intraperitoneal or oral administration 6-8% and 91-93% of the recovered mercury was excreted via urine and faeces, respectively.

Since the available PMA data did not give adequate information concerning absorption values, default values for oral absorption (50 %) and absorption via inhalation (100 %) were set in accordance with Guidance for the implementation of REACH chapter R.8 to derive the DNEL for PMA (ECHA, 2008a).

Grouping and read-across of the five phenylmercury compounds with regard to human health would theoretically rest upon the structural similarity and assumed similar toxicokinetic properties. Limited data is available, so during the elaboration of the restriction proposal the dossier submitter (Norway) approached two scientific institutes with the necessary skilled expertise with the aim of commissioning them to make a theoretical assessment of the probable absorption, distribution, metabolism and excretion in humans/mammals of the five phenylmercury compounds. The intention was that this could be done based on the substances´ chemical structure and similarity. Unfortunately the approached institutes were not able to take on this assignement. It should be noted that grouping and read-across weigh more heavily on the (environmental) degradation part, since due to the degradation to inorganic mercury species and subsequent biotransformation to methylmercury, the risk characterization (quantitative and qualitative) is mainly based on these compounds.

Metabolites, degradation products and transformation products

Oral ingestion of elemental mercury results in very limited absorption (<0.01% of dose), and the same is the case for dermal absorption of liquid elemental mercury (SCHER, 2008). In contrast, approximately 80% of the inhaled elemental mercury vapour is absorbed. Elemental mercury rapidly penetrates alveolar membranes due to its high lipid solubility (SCHER, 2008). Once absorbed, elemental mercury is readily distributed throughout the body, and it cross both placental and blood-brain barriers (EPA, 1997). The distribution of elemental mercury is limited primarily by the oxidation of elemental mercury to mercuric ion (Hg2+). Mercuric ion has limited ability to cross blood-brain and placental barriers. Once elemental mercury crosses the blood-brain barrier and is oxidized, return to the general circulation is hindered, and mercury can be retained in brain tissue (EPA, 1997). The elimination of elemental mercury and Hg2+ follow complex kinetics with half-lives in the range of 20 to 90 days (SCHER, 2008). After exposure to elemental mercury vapour the mercury may be excreted via exhaled air, urine, faeces, sweat and saliva (EPA, 1997). Only a small fraction of an ingested dose of inorganic mercury is absorbed from the gastrointestinal tract (SCHER, 2008). Hg^{2+} that is absorbed or formed by oxidation of elemental mercury may be eliminated by excretion with urine and/or faeces.

After ingestion of methylmercury most of an oral dose is absorbed from the gastrointestinal tract (about 95%) (SCHER, 2008). Inhaled methylmercury vapours are absorbed through the lungs (EPA, 1997). Methylmercury is distributed throughout the body and easily penetrates the blood-brain and placental barriers (UNEP, 2008). Estimates for the biological half-life of methylmercury range from 44 to 80 days (UNEP, 2008). In comparison, Magos (2003) computed a clearance half-time from whole blood of approximately 18 days for ethylmercury in adult humans. Faeces are the most important route for excretion of methylmercury as well as ethylmercury (SCHER, 2008; Clarkson and Mangos, 2006).

B.5.2 Acute toxicity

B.5.2.1 Non-human information

B.5.2.1.1 Acute toxicity: oral and intraperitoneal

Phenylmercury acetate
PMA is classified as Acute Tox. 3 in CLP Annex VI. The oral data in mice confirm this classification, see table Table B-27

Table B-27 Acute toxicity of phenylmercury acetate

Species	Administration route	LD50 mg/kg bw	Reference
Rat	Intraperitoneal	20	Eastman and Scott, 1944
Rat	Intraperitoneal	10	Swensson, 1952
Mouse	Intraperitoneal	20	Eastman and Scott, 1944
Mouse	Intraperitoneal	13	Swensson, 1952
Mouse	Oral	70	Goldberg *et al*., 1950
Rabbit	Intraperitoneal	5	Eastman and Scott, 1944
Chick	Oral	60	Miller *et al*., 1960

Phenylmercury propionate
No data found.

Phenylmercury octanoate
No data found.

Phenylmercury neodecanoate
No data found.

Phenylmercury 2-ethylhexanoate
No data found.

B.5.2.1.2 Acute toxicity: inhalation

No data found for any of the compounds.

B.5.2.1.3 Acute toxicity: dermal

No data found for any of the compounds.

B.5.2.2 Human information

Phenylmercury acetate

"Acute exposure to phenylmercuric acetate" (Goldwater et al., 1963)
Case report: A 26-years old male worker employed in a plant manufacturing a variety of mercurials, had no abnormalities prior to the accident. In an accident he was sprayed with a mixture of equal parts of benzene (benzol) and corrosive glacial (water free) acetic acid containing 12% (w/w) phenylmercuric acetate. Face, eyes, neck, arms and most of the clothing was soaked with the solution. He was immediately placed under an emergency shower and the contaminated clothing was removed. He was admitted to a hospital less than one hour after the accident occurred. Gastric lavage was preformed, and a cortisone-antibiotic preparation was applied to the eyes. The skin burns were treated with a nitrofurazone ointment. The only abnormalities seen at the time of hospital admission were second-degree burns of the face, ears, neck, arms, shoulders, and a small area on the right ankle. It was assumed that mercury had been absorbed through the skin and that some of the mix had been swallowed. The latter was confirmed when the stomach content was analyzed. The patient was given dimercaptopropanol (BAL) to promote the elimination of mercury and to minimize the toxic effects.
The only clinical symptoms observed were skin burns. Urine and blood samples were collected. The patient did not develop any signs of mercury intoxication except for a mild, transient albuminuria, which indicate some effect on the kidneys. It is difficult to evaluate the effect BAL had on the detoxification.
In the initial blood samples, all of the mercury was found in the red cells and none in the plasma. This proportion reversed itself in subsequent samples, suggesting that the mercury was absorbed as part of the PMA molecule.

Phenylmercury propionate
No data found.

Phenylmercury octanoate
No data found.

Phenylmercury neodecanoate
No data found.

Phenylmercury 2-ethylhexanoate
No data found.

B.5.2.3 Summary and discussion of acute toxicity

Phenylmercury acetate
Regarding to acute toxicity PMA is classified in EU as Acute Tox. 3; H301 – Toxic if swallowed (CLP regulation annex VI). This classification is supported by oral LD50 = 70 mg/kg bw in mice. For the case-report it is difficult to evaluate the effect of PMA since the worker was sprayed with and swallowed a mixture of benzene (benzol), glacial acetic acid and PMA.

Metabolites, degradation products and transformation products
Neurotoxicity is the most sensitive indicator of acute adverse effects in humans exposed to elemental mercury. As reviewed by EPA (1997), reports from accidental exposures to elemental mercury vapour have shown effects on cognitive, sensory, personality and motor

functions. Accidental exposure to high concentrations of elemental mercury vapour for a short period of time has caused mortality in humans due to respiratory failure (EPA, 1997). Urinary mercury concentrations in some of these studies indicated that body levels were up to 10 times higher than in controls (EPA, 1997). The kidney is a sensitive target organ following inhalation of elemental mercury vapour. Acute exposure may result in symptoms ranging from slight changes in urinary acid excretion to transient renal failure (EPA, 1997). The elemental mercury levels reported to be associated with preclinical and symptomatic neurological dysfunction are lower than those found to affect kidney and pulmonary function (EPA, 1997). Signs of cardiovascular effects have been observed after acute exposure of humans to elemental mercury vapour (EPA, 1997). In addition, acute high concentration exposure to elemental mercury vapour has been reported to cause gastrointestinal effects in humans (EPA, 1997). Exposure to elemental mercury vapours for acute or intermediate duration may also cause acrodynia or "pink disease", characterized by peeling palms, excessive perspiration, itching, rashes, joint pain and weakness, elevated blood pressure and tachycardia (UNEP, 2002). Regarding acute toxicity, elemental mercury is classified in EU as Acute Tox. 2; H330 – Fatale if inhaled (CLP regulation annex VI).

The kidney appears to be the critical target organ after ingestion of inorganic mercury (EPA, 1997). The estimated lethal dose of inorganic mercury for a 70 kg adult is 10-42 mg Hg/kg (EPA, 1997). Causes of death after ingestion of inorganic mercury include cardiovascular failure, gastrointestinal damage and acute renal failure (EPA, 1997).

B.5.3 Irritation

B.5.3.1 Skin

B.5.3.1.1 Non-human information

No data found for any of the compounds.

B.5.3.1.2 Human information

Phenylmercury acetate

No data found for any of the compounds.

B.5.3.2 Eye

B.5.3.2.1 Non-human information

No data found for any of the compounds.

B.5.3.2.2 Human information

No data found for any of the compounds.

B.5.3.2.3 Respiratory tract

B.5.3.2.4 Non-human information

No data found for any of the compounds.

B.5.3.2.5 Human information

No data found for any of the compounds.

B.5.3.3 Summary and discussion of irritation

Phenylmercuric acetate

There were some case reports indicated that PMA was an irritant (Morris, 1960; Biskind LH, 1951). However, in these studies very low doses were used, the data was not conclusive and the studies were incomplete reported. Hence, these reports were not included in this assessment. However, PMA is classified as a corrosive substance, which is a classification covering irritation as well (see B.5.4).

Metabolites, degradation products and transformation products

Red and burning eyes and conjunctivitis have been observed in persons exposed to high concentrations of elemental mercury vapours (WHO, 2003).

Dermal exposure to ionic mercury may lead to adverse effects to the skin, such as contact dermatitis (UNEP, 2008).

Case report studies suggest that dermal exposure to methylmercury in humans can cause rashes and blisters on the skin (ATSDR, 1999).

B.5.4 Corrosivity

B.5.4.1 Non-human information

Phenylmercury acetate

Investigations on the toxicity of some organic mercury compounds which are used as seed disinfectants (Swensson, 1952)

Mice given subcutaneous injection of 1 mg/ml PMA dissolved in water caused severe and widespread necroses of the skin. Due to animal welfare the experiment was not continued.

Comments: The study does not follow a guideline and is incomplete described.

Phenylmercury propionate

No data found.

Phenylmercury octanoate

No data found.

Phenylmercury neodecanoate

No data found.

Phenylmercury 2-ethylhexanoate

No data found.

B.5.4.2 Human information

No data found for any of the compounds.

B.5.4.3 Summary and discussion of corrosion

Regarding corrosion PMA is classified in EU as Skin Corr. 1B; H314 - Causes severe skin burns and eye damage (CLP regulation annex VI). It is reported that mice given PMA subcutaneously (the dose is not reported) showed severe and widespread necrosis of the skin and the experiment could not be continued. This finding indicates a corrosive effect of PMA. When a worker was accidently sprayed with a mixture of benzene (benzol) and glacial acetic acid containing 12% PMA, the exposure caused second degree burns. Glacial acetic acid has previously been classified in ECB as R34: Causes burns. Since PMA also has been classified as Skin Corr. 1B; H314, it is likely that the skin burns were caused by both glacial acetic acid and PMA (Goldwater *et al*., 1963, see Section B.5.2).

Metabolites, degradation products and transformation products

Inorganic salts of mercury are corrosive to the skin, eyes and gastrointestinal tract (WHO, 1991). Mercury dichloride and mercuric chloride are classified in EU (Table B-4 in Annex VI to CLP): Skin Corr. 1B; H314 – Causes severe skin burns and eye damage (Ex-EBC, 2010). Methylmercury is considered to be corrosive at high doses (WHO, 2000).

B.5.5 Sensitisation

B.5.5.1 Skin

B.5.5.1.1 Non-human information

No data found for any of the compounds.

B.5.5.1.2 2 Human information

Phenylmercury acetate

Contact urticaria syndrome due to phenylmercuric acetate (Torresani C. *et al*., 1993)
Case report: A 54-year old woman had eczema on both hands since 1973. In the last 2 years, she had experienced episodes of mild facial oedema, associated with rhino conjunctivitis and asthma. There was a positive family history of atopy. Analyses revealed a higher concentration of eosinophils and a higher titre of total IgE in the blood compared to normal levels. Open tests was carried out on her back. The patient displayed erythema (after 30 min) and urticaria (after 60 min) at the application site of PMA (0.01% in aqua solution). The reaction was associated with previous reported symptoms. Test of other mercurial compounds ruled out cross-reactivities. Open tests with PMA in three healthy control subjects gave negative results.

Allergic and non-allergic periorbital dermatitis: patch test results of the Information Network of the Departments of Dermatology during a 5-year period (Herbst R. A. et al., 2004).

Materials and Methods: Patch test results used in this study are from the Information Network of the Departments of Dermatology (IVDK). IVDK is an instrument of epidemiological surveillance of contact allergy, and is described by Uter *et al*. (1998). Information is available online (http://www.ivdk.org/). IVDK is a database which comprises patch test data from all patients tested in 32 centers in Germany and Austria from 1995 to 1999. A total of 49256 patch-tested patients have been included. Patch tests were performed to confirm or exclude contact allergy and were done according to international guidelines. PMA 0.05% was one of the compounds in the test battery. Among the patients 1053 (2.1%) were diagnosed as allergic periorbital contact dermatitis (APD), 588 (1.2%) as non-allergic periorbital dermatitis (NAPD). Other Cases (OC) were the remaining patients. APD and NAPD were constituted by approximately 80% female, and 68% and 53% were above 40 years, respectively.
Results: 892 of the APD patients were tested for PMA and 9.2% responded positive. Among the NAPD patients (490) only 5% responded positive and for OC patients 6.7% responded positive to PMA, as outlined in the table below.

Table B-28 Patch test results for PMA

	APD			**NAPD**			**OC**		
	Number of patients	Standard PT positive	95% CI standard PT positive	Number of patients	Standard PT positive	95% CI standard PT positive	Number of patients	Standard PT positive	95% CI standard PT positive
PMA	892	9.2%	7.1-11.3	490	5.0%	3.1-6.9	27649	6.7%	6.4-7.0

PMA: Phenylmercuric acetate 0.05%

Topically applied ophthalmic drugs are a potential cause of allergic contact dermatitis of the periorbital region. The proportion of positive reactions to PMA was significantly ($p>0.05$) higher in APD compared to that in OC. Even when the proportion of positive reactions was adjusted for age and sex differences, the response in the APD was significantly higher than in OC. Thus, PMA was suggested to be a true ophthalmic allergen.

Patch testing with phenylmercuric acetate (Geier J. et al., 2005)
Materials and methods: From December 2002 to June 2004 a total of 1151 patients, with suspected exposure to one of the allergens in the patch test, were included in this study. This study was performed by the German Contact Dermatitis Research Group (DKD). The concentrations of the PMA solutions in the patch tests were 0.05% and 0.01%.

Results:
Table B-29 Patch test reactions at day 3 to PMA

	Test concentration	
Reaction at day 3	0.05%	0.01%
Negative	905	1137
?	81	2
+	97	9
++	18	1
+++	6	0
Irritant	44	2
Total	1151	1151

PMA 0.05% caused positive response in 10.5% (n=121) of the patients and doubtful or irritant reactions in 10.9% (n=125). The reaction index (RI) was -0.02 which indicate that it is

difficult to conclude whether the PMA gives rise to sensitisation or irritation/doubtful reactions. (RI is defined as the ratio of positive patch test reactions minus questionable and irritant reactions divided by the total sum of these reactions). With 97+ reactions among a total of 121 positive reactions, the positive ratio (PR) was 80%. (PR is defined as the frequency of + reactions among the total number of positive patch test reactions (+ to +++)).

For PMA 0.01% only 10 patients (0.9%) reacted positively. Nine of these gave a + reaction. Hence, the PR was 90%. Doubtful or irritant reactions occurred in 4 patients (0.35%) and gave an RI of 0.43.

Of the 10 patients reacting positively to PMA 0.01%, only 4 had a simultaneously positive test reaction to PMA 0.05%, while in the other 6 patients, the patch test with PMA 0.05% remained negative. The proportions of positive reactions to the two test concentrations differed significantly ($p < 0.0001$). Of the 24 patients with a strong reaction (++,+++) to PMA 0.05%, 22 did not react to PMA 0.01% at all.
One would expect that patients allergic to PMA, with a positive reaction to the lower test concentration, would be expected to react positively to the higher concentration as well, presumably with a stronger response. These results indicate that by far not every positive reaction to PMA is truly allergic. For the PMA 0.05%, positive patch test and irritation was observed in ~ 14% of the patients, 7% of all the reactions were doubtful and 79% of the patients were tested negative.

An additional comparison of test reactions to PMA and two other organic and inorganic mercury compounds (thimerosal and mercury amide chloride) revealed no cross reactivity. Data on clinical relevance of positive test reactions were not available.

Contact hypersensitivity to selected excipients of dermatological topical preparations and cosmetics in patients with chronic eczema (Dastychová E. *et al*., 2008)
Materials and methods: Contact sensitization to selected excipients of dermatological topical preparations and cosmetic were tested on 1927 patients with chronic eczema (mean age 44.3 years, 601 males, 1326 females). PMA 0.05% was tested. The reaction was scored 3 days after application.

Results: Patch tests indicated that 3.1% of the patients were sensitized to PMA. Thiomersal is a sodium ethylmercurithiosalicylate and is a known allergen. For thiomersal 11.3% responded positive and the authors suggested that the response to PMA may be caused by cross-sensitivity to thiomersal.

Phenylmercury propionate
Immediate type hypersensitivity to phenylmercuric compounds (Mathews *et al*., 1968)
Case report: A 34-year old male resident physician experienced symptoms of asthma and urticaria. He had a family history of asthma and as a child he had food allergy and rhinitis symptoms. After taking a position at the University Hospital he developed a progressive rhinitis and for the first time asthma symptoms. The symptoms were immediate type of hypersensitivity. Phenylmercuric propionate used in the fabric softener (0.85%) used by the University Laundry was found to be the trigger factor for these symptoms.

Phenylmercury octanoate
No data found.

Phenylmercury neodecanoate
No data found.

Phenylmercury 2-ethylhexanoate
No data found.

B.5.5.2 Respiratory system

B.5.5.2.1 Non-human information

No data found for any of the compounds.

B.5.5.2.2 Human information

No data found for any of the compounds.

B.5.5.2.3 Summary and discussion of sensitisation

Phenylmercury acetate
In a large database of patch test data, 9.2% of the patients with periorbital contact dermatitis testes positive to PMA. Only 5- 6.7% of patients that had non-allergic perorbital contact dermatitis or were defined as "other cases", tested positive to PMA. The authors suggest that the finding indicates that PMA is an ophthalmic allergen. Cross-sensitivity to other mercury compounds has been suggested. Moreover, it has been discussed whether PMA is a sensitizer or an irritant compound. In one study where patients were patch tested for PMA it was difficult to conclude whether the compound was a sensitizer or not. Most of the responses due to sensitisation were weak (+). Contact urticaria syndrome due to PMA has been described in a case report.
In conclusion, the results from the available studies are inconclusive and PMA would most likely not be classified in EU based on these data. It is also difficult to rule out the possibility that the responses are caused by irritations or whether there is cross-reactivity involved.

Phenylmercury propionate
A case report describes a patient with severe immediate type hypersensitivity to phenylmercuric propionate.

Metabolites, degradation products and transformation products
Contact dermatitis may develop as a result of acute or occupational exposure to inorganic mercury. Patch tests conducted in many of the cases show some cross-reactivity between various inorganic and organic forms of mercury (ATSDR, 1999).

B.5.6 Repeated dose toxicity

B.5.6.1 Non-human information

B.5.6.1.1 Repeated dose toxicity: oral

Phenylmercury acetate

Phenylmercuric acetate as a contraceptive (Nicholson et al., 1944)
Materials and methods:
Three animal experiments were performed and reported in this study. Human data is reported in Section B.5.1.

Experiment 1: Groups of 6 rats (bw approximately 60 g, strain was not reported) were given 2 or 4 mg/kg bw PMA intraperitonally five days a week for two weeks (corresponds to 10-20 mg PMA/kg bw/w).
Experiment 2: Four rabbits (bw not given) were administrated an intravenous injection of 1 mg/kg bw PMA five days a week for two weeks (corresponds to 5 mg PMA/kg bw/w).
Experiment 3: Groups of eight rabbits (bw not given) were given 0.1 or 0.2 mg/kg bw PMA intraperitonally five days a week for ten weeks (corresponds to 0.5-1.0 mg PMA/kg bw/w).

Comment: These experiments do not follow test guidelines and are incomplete described. Data for several endpoints are lacking.

Results: For all the experiments weight records, blood counts and urine examination showed no abnormalities or signs of toxicity. Histopathological examinations were made of the liver, kidney, spleen and adrenal gland of all animals. No significant deviation from the normal histological picture was encountered.

"Distribution and excretion of methyl and phenyl mercury salts" (Gage, 1964)
Material and Methods: Female albino Wistar rats (bw 125-135g) were injected subcutaneously three times a week for up to six weeks with an aqueous solution of PMA. The dose was equivalent to 0.15 mg mercury/rat (0.45mg mercury/week which corresponds to 0.76 mg PMA/week for six weeks) which resulted in a total dose of 2.7 mg mercury/4.5 mg PMA. By using the mean body weight of the rats at the beginning of the experiment (130 g) the dose of PMA was 5.8 mg/kg bw/w.

Comment: The weight of the rats was low and may indicate young animals. The age was not reported. The study is general incompletely described and data for several endpoints are lacking.

Results:
At the end of the six week period the body weight range for the treated animals was 170 to 190 g. No toxic effects were observed after treatment with the equivalent of 5.8 mg PMA/kg bw/w for six weeks, and no measurable accumulation of mercury was found in the central nervous system.

"FAO Meeting Report No. PL/1965/10/1 WHO/Food Add./27.65"
Materials and methods "A rabbit was fed with a diet containing PMA for 130 days, the total amount of mercury consumed during the experimental period being 770 mg. The animal showed marked growth depression and died after 130 days. Chemical analysis revealed large amounts of mercury in the organs - 29 mg/kg organ-weight in the kidney, 0.52 mg/kg in the liver and 5.18 mg/kg in the gastro-intestinal tract - whereas a control rabbit showed only 0.06 mg/kg in the kidney and traces in the liver. Another rabbit fed a diet containing PMA for 100 days received a total amount of 6.9 mg of mercury. There was no abnormality in appearance

or growth. The contents of mercury in the organs were 0.455 mg/kg in the kidney and 0.042 mg/kg in the liver.
A guinea-pig was fed a diet containing PMA for 670 days and consumed a total of 20.4 mg mercury during the whole experimental period. No ill-effects were observed in general appearance or growth. The mercury content of the kidney was 4.76 mg/kg organ-weight, whereas that of a control animal was 0.3 mg/kg"

Investigations on the toxicity of some organic mercury compounds which are used as seed disinfectants (Swensson, 1952)
Rats were given intraperitoneal injections of PMA at dosages of 1-2.5 mg/kg body-weight every other day for 4 weeks. The animals showed gradually increasing apathy and loss of weight. This was explained by the strongly irritating effect upon the peritoneum by the author. There were findings of diffuse cell injures in the cerebellum and spinal cord. The injuries were of the same type for several alkylmercury compounds and PMA and it was not possible to show any essential differences in the different substances tested. Thus, we question these findings.

Comments: The dose 1-2.5 mg/kg bw/injection corresponds to 3.5-8.75 mg/kg bw/w.

"Chronic oral toxicities of mercuri-phenyl and mercuric salts" (Fitzhugh et al., 1950)
Materials and methods: Groups of 10-12 rats of both sexes (initial bw 50 g, strain not reported) were fed diets containing 0.1, 0.5, 2.5, 10, 40 and 160 ppm of mercury as PMA or mercury acetate for up to two years. In addition there were two control groups of twenty rats each. The mercury salts were added to the basic diet. The animals were fed ad libitum and body weights and food consumptions were measured weekly. At two separate times, at six months and one year, urine and faeces were separately collected over a 24-hours period from members of each group and analysed for mercury. At the age of one year, two males and females from each group were killed and their liver and kidney were analysed for mercury. Terminal analyses were made on nearly all the animals that died between the ages of 18 months and two years. Of the 284 rats started on these experiments, 197 were examined in the pathology laboratory. Forty-five rats were examined microscopically in a detailed manner. In essentially every instance, sections were made of the following structures: Lungs, heart, liver, spleen, pancreas, stomach, small intestine, colon, kidney, adrenal gland, thyroid gland, testis (or uterus and ovary), leg muscles, leg bones and bone marrow. Brain and skin were sectioned in four instances and a number of lymph nodes and parathyroid glands were incidentally sectioned. In 98 additional instances sections were made only of liver, kidney and (in males) testis.No data was shown for the histopathological examination in the paper.

Comment on study quality: The study is not performed in accordance with the OECD test guideline 452. The main deviations are reduced number of animals in the groups (10-12/sex in the study, while 20 is recommended in the guideline) and incompletely described results.

Results: Exposure to PMA at dosage level of 160 ppm mercury reduced the average survival period. No animal in the group survived as long as 18 months. At other dosage levels no increase in mortality was observed.
Only male rats exposed to 10 ppm mercury as PMA for 52 weeks had retarded growth compared to the controls, whereas 40 ppm mercury as PMA significantly retarded the growth of both sexes. No growth retardation was observed for the groups exposed to mercury given as mercury acetate in the same period of time. The food consumption was not affected in any groups.

Both mercuric acetate and PMA at dosage levels of 40 and 160 ppm mercury produced significant enlargement of the kidneys. The mean weight of kidneys to rats exposed to 0.5 ppm mercury as PMA were also significantly increased compared to that of the controls. The livers of animals given 40 or 160 ppm were slightly higher compared with the controls.

Table B-30 Mean liver and kidney weights of rats fed mercuric acetate or PMA for 12 months

Compound	Dietary mercury level (ppm)	Animal	Liver (g/kg bw)	Kidney (g/kg bw)
Control	0	5	38.5±3.9	10.5±1.0
Mercuric acetate	0.5	5	35.9±5.5	9.4±0.8
	2.5	6	33.5±2.8	11.5±1.7
	10	4	35.2±3.9	9.9±1.3
	40	7	41.0±4.7	14.2±1.2*
	160	6	42.1±1.9	14.8±1.6*
PMA	0.1	9	34.9±2.0	11.8±1.2
	0.5	6	37.0±2.8	15.5±2.0*
	2.5	5	31.4±3.2	13.8±2.7
	10	7	33.1±2.3	10.9±1.0
	40	3	40.2±6.1	25.5±6.2*
	160	1	40.0	13.3*

*$p < 0.05$

An interesting observation was that PMA in the diet caused 10 to 20 times more mercury stored in the liver and kidney tissue compared with the level stored when the rats were exposed to mercury acetate. Also, it was found a tendency for more mercury (given as PMA) to be stored in the liver with increasing exposure time. The same tendency was not observed for the kidneys. It should be emphasized that this was based on a limited number of animals and thus only at 0.5 ppm the accumulation in liver was found significantly higher ($p \approx 0.05$) after two year of exposure.

Table B-31 Average storage of mercury in the liver and kidney of rats fed mercuric acetate or PMA for a period of twelve months

Compound	Dietary mercury level (ppm)	Liver (µg Hg/g wet tissue)	Kidney (µg Hg/g wet tissue)
Control	0	0.01	0.14
Mercuric acetate	0.5	0.05	0.60
	2.5	0.07	2.6
	10	0.14	2.5
	40	0.33	16
	160	0.54	40
PMA	0.1	0.05	1.7
	0.5	0.14	17
	2.5	0.57	27
	10	1.5	40
	40	14	48

	160	31	37

Average of four animals in each group.

Table B-32 Average storage of mercury in the liver and kidney of rats fed mercuric acetate or PMA for a period ranging from eighteen months to two years

Compound	Dietary mercury level (ppm)	Liver (µg Hg/g wet tissue)	Kidney (µg Hg/g wet tissue)
Control	0	0.07	0.28
Mercuric acetate	0.5	0.07	0.61
	2.5	0.18	1.1
	10	0.33	4.6
	40	0.92	10
	160	1.4	48
PMA	0.1	0.25	2.3
	0.5	0.43	4.6
	2.5	0.83	30
	10	3.3	39
	40	21	19
	160	-	-

Average of two to six animals in each group. The groups represent the animals which died at age from 18 months to 2 years.

Levels of mercury in urine and faecal excretion were measured in a 24 hour period after 6 and 12 month of exposure. The urinary excretion was decreased with increasing dose level and was found to be higher in the groups given mercury as PMA compared to the groups given mercury acetate. At 0.5 ppm mercury given as PMA and mercury acetate, 9.2 % and 4.8% of the dose was excreted in urine, respectively.

Table B-33 Twenty-four hour excretion of mercury by rats fed PMA or mercuric acetate.

		PMA				Mercuric acetate			
		Urinary excretion		Faecal excretion		Urinary excretion		Faecal excretion	
Dietary level ppm	24 hours average µg	Total µg*	% of intake	Total µg*	% of intake	Total µg*	% of intake	Total µg*	% of intake
0.5	7.5	0.79	9.2	3.3	44	0.36	4.8	3.9	52
2.5	37.5	1.7	4.5	13	35	0.39	1.0	15	40
10	150	9.3	6.2	40	27	0.76	0.5	64	43
40	600	26	4.3	209	35	2.2	0.37	284	47
160	2400	57	2.4	490	20	4.1	1.7	1027	43

*The total represents the average of 9 to 12 animals at each level of intake.

Gross pathological examination revealed enlargement, fibrosis and granularity of the kidney, hairballs in the stomach and moderate paleness of the viscera suggesting anaemia at 0.5 ppm and upward. Enlargement, fibrosis and granularity of the kidney also occurred in the control

animals, but later and less intensely compared with the animals administrated PMA. Hairballs in the stomach and paleness of the viscera were observed in less than 5% of the treated animals. These effects were not observed in the control animals.

In the first half of the experimental period a considerable number of animals died from massive pneumonia. This could not be related to the dosage of mercury. Two animals in the high dose group had extensive inflammatory involvement of the cecum. The remaining occasional lesions (arthritis, tremors, testicular atrophy, etc) showed no correlation with treatment.

Microscopic observations were performed in 45 rats. Severe damage of the kidney tubules was demonstrated. Hypertrophy and dilatation of the proximal convoluted tubules in the inner half of the cortex, with various epithelial changes was observed. As the lesion progressed the dilated tubular segment became larger, hyaline casts appeared within them and within other tubules in both the medulla and the outer half of the cortex. Some tubular segment atrophied and fibrosis and a slight to moderate chronic cellular inflammatory infiltration occurred. A further progression of the lesions resulted in development of cysts of the dilated tubular segments and cortical fibrosis. The severity of renal damage is given in Table B-34.

In seven animals the bone marrow revealed a slight normoblastic hyperplasia, which was accompanied with similar change in the spleen. In the paper there is no information concerning which animals these findings was observed in. Microscopic examination of the two animals in the high dose group with extensive inflammation in the cecum, thickened, necrotic walls and extensive, shallow ragged ulceration was found, while their stomach appeared as normal. In addition, in one of these animals focal calcification in heart and leg muscles was observed. This finding may be more related to the gastrointestinal effect rather than by the PMA it selves. No effects on heart and leg muscles were observed in any other animals. Liver, testis, thyroid gland, lung, pancreas, small intestine, colon, adrenal gland, uterus, ovary or leg bone was not affected by PMA.

Table B-34 Comparative kidney damage in rats ingested PMA and mercury acetate

Renal damage					
		Females		Males	
Compound	Dose level Hg ppm	One year group	Entire group	One year group	Entire group
Control	0	Non	Slight	Non	Very slight
PMA	160	Marked	Marked	Marked	Marked
	40	Marked	Marked	Very slight	Moderate to slight
	10	Marked	Marked	None	Slight
	2.5	Slight	Moderate	None	**Slight**
	0.5	Very slight	**Moderate**	None	Very slight
	0.1	None	Slight	None	Very slight
Mercury acetate	160	Moderate	Moderate to marked	Slight	Slight to moderate
	40	Very slight	Slight to moderate	Very slight	Slight

	10 or less	None	Slight	None	Very slight

These results indicate that PMA is more toxic to rats than mercury acetate. The dose level of 0.5 ppm mercury as PMA resulted in detectable kidney damage in females after 2 years. No differences were seen between controls and females receiving 0.1 ppm mercury. At 2.5 ppm renal lesions were observed in the males. Based on these results a NOAEL of 0.1 ppm is established. The EPA has assumed that the rats consume about 5% of their body weight in food per day and a body weight default value of 375 g was used to convert 0.1 ppm into 0.0084 mg PMA/kg bw/day (EPA, 2010).

Phenylmercury propionate
No data found.

Phenylmercury octanoate
No data found.

Phenylmercury neodecanoate
No data found.

Phenylmercury 2-ethylhexanoate
No data found.

B.5.6.1.2 Repeated dose toxicity: inhalation

No data found for any of the compounds.

B.5.6.1.3 Repeated dose toxicity: dermal

No data found for any of the compounds.

B.5.6.1.4 Repeated dose toxicity: other routes

No data found for any of the compounds.

B.5.6.2 Human information

No data found for any of the compounds.

B.5.6.3 Summary and discussion of repeated dose toxicity

Phenylmercuric acetate
Target organ for sub-chronic and chronic exposure to PMA in rats, rabbits and guinea-pig is the kidney. In all studies where the mercury levels were measured, mercury was found to accumulate in this tissue.

In sub-acute experiments, rats administrated (ip) 10 or 20 mg PMA/kg bw/w and rabbits administrated (iv) 5 mg PMA/kg bw/w for two weeks showed no effect of the treatment. Subcutaneously administration of PMA to rats for six weeks (5.8 mg PMA/kg bw/week) did not caused any effects. Also when rabbits were exposed for teen weeks to PMA at lower dose (ip, 0.5 – 1.0 mg/kg bw/w) no effect of the treatment was reported. However, when rats were given PMA intraperitonal for four weeks (3.5-8.75 mg PMA/kg bw/w), increased weight loss and apathy were observed. No neurological effect of PMA has been reported in other studies described in this report.

Chronic oral exposure of female rats to PMA from 0.5 ppm mercury (0.042 mg PMA/kg bw/d correspond to 0.29 mg PMA/kg bw/w) in the diet caused enlargement of the kidneys and moderate kidney damage (e.g., tubular dilation, atrophy, granularity, fibrosis). No differences in renal damages were observed between controls and females receiving 0.1 ppm mercury (correspond to 0.0084 mg PMA/kg bw/d or 0.059 mg PMA/kg bw/w). At higher doses renal lesions were observed in both males and females. At all dose levels exposed animals accumulated mercury in the kidney and liver. The females seem to be more susceptible than the males. Based on these results a NOAEL of 0.1 ppm (corresponding to 0.0084 mg PMA/kg bw/day), is suggested by the EPA (EPA, 2010). The Norwegian Institute of Public Health supports this NOAEL.

PMA is classified in EU (Table B-4 in Annex VI to CLP): STOT RE 1; H372 – Causes damage to organs through prolonged or repeated exposure (Ex-ECB, 2010).

Metabolites, degradation products and transformation products

Neurological and behavioural disorders in humans have been observed following inhalation of elemental mercury vapour (UNEP, 2002). As reviewed by EPA (1997), studies of populations chronically exposed to potentially high concentrations of mercury vapour have shown altered sensory, cognitive, personality and motor functions. One characteristic symptom after long-term high dose exposures (inhalation of concentrations above 0.5 mg/m3 for many years) is muscle tremors, which may progress to chronic spasm of the extremities (SCENIHR, 2008). It was concluded in a recent assessment of all studies on the exposure-response relationship between inhaled mercury and adverse health effects that several studies consistently demonstrate subtle effects on the central nervous system after long-term occupational exposure. These effects were observed at exposure levels of around 20 μg/m3 and higher (WHO, 2003). The kidney is, together with the central nervous system, a critical target organ after exposure to elemental mercury vapour (UNEP, 2002). After chronic exposure to elemental mercury vapour, proteinuria and nephritic syndrome have been described in humans. The glomerular damage may progress to interstitial immuno-complex nephritis (SCENIHR, 2008). Elemental mercury can be oxidized to Hg^{2+} in the kidneys, and the kidneys accumulate this inorganic mercury to a larger extent than most other tissues (UNEP, 2002). Kidney concentration of mercury in occupationally exposed groups is typically around 0.1-0.3 μg/g (UNEP, 2002). Long-term oral administration of Hg^{2+} to rodents cause glomerulonephritis, which was caused by altered immuneresponses, thus being similar to the human effects described after long term inhalation of elemental mercury (SCENIHR, 2008). Elemental mercury and mercury dichloride and mercuric chloride are classified in EU (Table 3.1 in Annex VI to CLP): STOT RE 1; H372 – Causes damage to organs through prolonged or repeated exposure (Ex-ECB, 2010).

The critical target organ for methylmercury toxicity is the nervous system, particularly during development. In adults, the earliest effects of methylmercury poisoning are symptoms such as paresthesia, discomfort, and blurred vision. At higher exposure the following symptoms may appear; disturbances of the visual field, deafness, dysarthria, ataxia, and ultimately coma and death (UNEP, 2002). The developing nervous system is more sensitive to methylmercury than the adult nervous system. Offspring from mothers consuming methylmercury contaminated food during pregnancy have shown a variety of developmental neurological abnormalities including microcephaly, hyperreflexia, and gross motor and mental impairment (UNEP, 2008: UNEP 2002). Some studies suggest that small increases in methylmercury exposure may cause adverse effect on the cardiovascular system, including increased risk of acute myocardial infarction and elevated blood pressure (UNEP, 2002; UNEP 2008). However, WHO has concluded that the available evidence on this endpoint is not conclusive (FAO/WHO, 2004). TC C&L have proposed the following classification for methylmercury: T; R48/25: Toxic: danger of serious damage to health by prolonged exposure if swallowed (Ex-ECB, 2010).

B.5.7 Mutagenicity

B.5.7.1 Non-human information

B.5.7.1.1 In vitro data

Phenylmercury acetate

Distinct genotoxicity of phenylmercury acetate in human lymphocytes as compared with other mercury compounds (Lee C. *et al*., 1997; Lee C. *et al*., 1998).

Two studies have been conducted on PMA on human lymphocytes measuring the frequency of sister chromatid exchanges (SCEs).

Materials and Methods: The frequency of SCEs was assayed to evaluate the genotoxic effects of PMA on human lymphocytes from five healthy males. The tested doses were 0, 1, 3, 10, 20, 30 µM PMA and 0.15 µM mitomycin C (MMC) as positive control. The study was performed largely according to the OECD 479 test guideline. Endoreduplication was also recorded.

Results: PMA (1-30 µM) increased the frequency of SCE in a concentration-dependent manner, and a statistically significant dose-related increase in the mean number of SCEs per cell was observed from 10 uM PMA. PMA also increased the frequency of endoreduplicated mitosis in a concentration-dependent manner.

Table B-35 Effects of PMA on SCE and proliferating rate index (PRI) in cultured human lymphocytes (Lee C. et al., 1997)

Treatment	Concentration (µM)	Number of metaphase	SCEs/cell (mean ± SE)	PRI [a] (mean ± SE)
Control	–	250	7.0 ± 0.4	2.25 ± 0.05
MMC	0.15	200	49.5 ± 0.6 [b]	1.51 ± 0.04 [b]
PMA	1.00	250	6.9 ± 0.3	2.32 ± 0.11
	3.00	250	7.4 ± 0.4	2.15 ± 0.08
	10.00	250	9.5 ± 0.4 [b]	1.90 ± 0.06 [b]
	20.00	250	13.0 ± 1.1 [b]	1.74 ± 0.04 [b]
	30.00	250	14.9 ± 0.6 [b]	1.62 ± 0.03 [b]

[a] PRI was calculated according to the following formula [26]: $PRI = 1M_1 + 2M_2 + 3M_3/100$. For each treatment group three replicate cultures were assessed.

[b] $p < 0.05$ as compared with control

Table B-36Effects of phenylmercury acetate on sister exhanges (SCE) and proliferating rate index (PRI) in cultured human lymphcocytes *(Lee C.et al, 1998)*

Treatment	Concentration (µM)	Number of metaphases	SCE per cell (mean ± S.E.)	PRI[a] (mean ± S.E.)
Control	—	120	7.2 ± 0.2	2.32 ± 0.08
MMC	0.03	120	18.0 ± 0.1*	1.65 ± 0.05*
PMA	20	120	14.5 ± 0.5*	1.70 ± 0.07*

[a]PRI was calculated according to the following formula [Lamberti et al., 1983], three replicate cultures were assessed for each treatment group: $PRI = (1M_1 + 2M_2 + 3M_3)/100$.

*$P < 0.05$ as compared with control.

Mitomycin C (MMC) was used as a positive control.

Phenylmercury propionate

No data found.

Phenylmercury octanoate
No data found.

Phenylmercury neodecanoate
No data found.

Phenylmercury 2-ethylhexanoate
No data found.

B.5.7.1.2 In vivo data

No data found.

B.5.7.2 Human information

Chromosome distribution studies in phenylmercury acetate exposed subjects and in age-related controls (Verschaeve L. *et al*., 1978).
Peripheral blood lymphocytes of PMA exposed persons and a control population of the same age were evaluated for chromosomal distribution changes.
Materials and Methods: Blood samples were taken from well-protected PMA exposed persons who are estimated to handle 20-30 kg mercury a few times a week and age-matching control groups. Within 24 h after collection of the blood, peripheral lymphocytes were cultured for 48 h in the presence of colchicine. A total of 100 metaphase plates were studied for the mercury exposed persons (16 male individuals: 12 with 5 metaphases each and 4 individuals with 10 metaphases) as well as for the controls (12 male individuals: 4 with 5 metaphases each and 8 with 10 metaphases). Mercury levels in the blood were analyzed using analytical methods (a flameless atomic absorption technique) in both exposed and control groups.
Results: Mercury levels in the blood were ranging between 0 and 3.5 µg/1 in the control population (mean: 0.84 µg/l) and between 0 and 5.6 µg/1 (mean: 2.32 µg/1) in the exposed group. All values were thus within the normal (<5 µg/1 accepted as normal). With respect to metaphase cytogenetic analysis the PMA-exposed subjects do not differ from the controls. In the PMA-exposed subjects no differences in aneuploidy or hypoploidy were observed but there were a small statistically significant increase in hyperploidy, and no translocations could be detected. The significance of this finding is difficult to establish since the other parameters did not show any effect. Distance to the metaphase plate centre (d2) and distance between homologous and non homologous chromosome combinations were analyzed (Δ2). No chromosomes had a statistically significant difference in d2 except chromosomes 16 ($0.025 < p < 0.05$). For the mercury group the tendency to migrate from each other is expressed (Δ2). However only the pairs 15–18 and 17-22 become significantly less associated. The exposure level was extremely low, and remarkable modifications in the chromosome distribution as compared with a control group would hardly be expected. This was indeed not found, although some results seem to be of particular interest. The study concludes on a weak alteration in the chromosome distribution in the mercury-exposed population, i.e. a possible implication of mercury in the nucleolar activity.

B.5.7.3 Summary and discussion of mutagenicity

Phenylmercury acetate

Two in vitro studies showed that exposure to PMA causes SCE, and also induced high frequency of endoreduplication in cultured human lymphocytes (Lee C. *et al*., 1997; Lee C. *et al*., 1998). PMA has been found to elevate the frequency of micronuclei in the root cells of Allium (Dash S. *et al*., 1988). Human data indicates a weak alteration in the chromosome distribution in the PMA-exposed population, i.e. a possible implication of mercury in the nucleolar activity, although with extremely low exposure level. At this exposure level an increased frequency of hyperploidy was observed.

Based on these data PMA may be mutagenic, but the existing data are insufficient for classification as a mutagen.

Metabolites, degradation products and transformation products

Findings from genotoxicity assays are limited and do not provide supporting evidence for a mutagenic effect of elemental mercury (UNEP, 2008).

There is some evidence that mercuric chloride may be a germ cell mutagen. Positive results have been obtained from chromosomal aberration assays in multiple systems, and evidence suggests that mercuric chloride can reach female gonadal tissues (UNEP, 2008). Mercury dichloride and mercuric chloride are classified in EU (Table B-4 in Annex VI to CLP): Muta. 2; H341 – Suspected of causing genetic defects (Ex-ECB, 2010).

Data from several studies in humans suggest that oral exposure to methylmercury may cause chromosomal aberrations and SCE (UNEP, 2002). Studies have shown evidence that methylmercury may induce mammalian germ cell chromosome aberrations (EPA, 1997). Regarding mutagenicity TC C&L has agreed on the following classification for methylmercury: Muta. Cat. 3; R68: Possible risk of irreversible effects (ClassLab, Ex-ECB, 2010).

B.5.8 Carcinogenicity

B.5.8.1 Non-human information

No data found for any of the compounds.

B.5.8.2 Human information

No data found for any of the compounds.

B.5.8.3 Summary and discussion of carcinogenicity

No data were found for any of the phenylmercury compounds.

Metabolites, degradation products and transformation products
Based on the overall evaluation of the International Agency on Cancer (IARC) elemental mercury and inorganic mercury are not classifiable as carcinogenic to humans (group 3) (UNEP, 2002). Methylmercury compounds are considered possibly carcinogenic to humans (group 2B) according to IARC, based on their overall evaluation (UNEP, 2002). The classification proposed by the TC C&L for methylmercury regarding carcinogenicity is as follows: Carc. Cat. 3; R40: Limited evidence of a carcinogenic effect (ClassLab, Ex-ECB, 2010).

B.5.9 Toxicity for reproduction

B.5.9.1 Non-human information

Phenylmercury acetate
Embryonic susceptibility of Microtus ochrogaster (common prairie vole) to phenylmercuric acetate (Hartke et al., 1976)
Materials and methods: To evaluate the maternal toxicity of PMA ip LD50 was determined by using 24 adult M. ochrogaster females.
Oestrus was induced by placing a mature male and mature female in a "smell cage". When the divider was removed, copulation usually occurred within minutes. The presence of a vaginal plug was used to confirm mating. A total of 74 pregnant M. ochrogaster were administrated a single intraperitoneal doses of 0.06, 0.125, 0.5, 1, 2, or 5 mg/kg bw PMA on day 8 (n=25), 9 (n=32) or 10 (n=16) of gestation. PMA was dissolved in double distilled water and the volume used was 1 ml/100g bw. Control animals received 1 ml of double distilled water/100g bw. Eight other females were administrated 0.5 mg/kg bw PMA on day 7, 11 or 12 to determine dose-stage relationship.

All animals were sacrificed on day 16 of gestation to count corpora lutea, number of live foetuses and number of resorption sites. All of the morphological features used for teratological evaluation are well developed. Dead or malformed foetuses are readily recognizable by the sixteenth day. Most gross morphological features are easily distinguishable and documented. Resorption site were still grossly detectable. Animals were euthanatized with sodium pentobarbital and their reproduction tracts removed. Foetuses, uteri, and ovaries were examined under a dissecting microscope before and after fixation (10%

buffered neutral formalin). Histological sections were made of uteri with resorption site and of random embryos surviving in the same organ. Tissues were embedded in paraffin, sectioned at 7 μm, and stained with hematoxylin and eosin.

Comments: In this study only the effect of PMA on development of foetuses was examined, and not effects on fertility and maternal behaviour. The study design is not in accordance with OECD test guidelines for reproduction toxicity studies.

Results: The ip LD50 for PMA for adult M. ochrogaster was 10 mg/kg bw.
At day 8 (embryo age) a maternal dose of 0.125 mg/kg bw caused 33% resorption. Compared to the control, this is a five fold increase of resorption (% of the litters). At day 10 the resorption did not increase (40%) before the mice were given 0.5 mg/kg bw. In this study PMA was found to be 100% embryo-lethal at dosage of ≥ 1 mg/kg bw. High incidence of intrauterine embryonic deaths and resorption was found to be dose and stage of embryo development dependent. The effect increased with increasing dose (Table B-37) and decreasing embryo age (Table B-38). No structural abnormalities were found in any of the foetuses in control or treated groups.

Histopathological sections: No histological findings were observed in liver, kidney and hair of all animals.

Table B-37 Embryo susceptibility to PMA in 8-, 9-, and 10 day Microtus ochrogaster embryos

Embryo age	Maternal dosage (mg/kg)	Average number of corpora lutea	Average number of live foetuses	Average number of preplacentation losses	Average number of postplacentation losses	Average pre- and postimplatation loss (% of litter)
8	0	4.50	4.25	0.25	0.00	6
	0.06	4.00	4.00	0.00	0.00	0
	0.125	3.00	1.00	0.38	1.63	33
	0.25	5.00	1.75	0.50	2.75	65
	0.5	3.80	1.00	0.40	2.40	74
	1	4.00	0.00	0.00	4.00	100
	2	4.00	0.00	0.50	3.50	100
	5	4.50	0.00	0.50	4.00	100
9	0	4.00	4.00	0.00	0.00	0
	0.06	4.25	3.75	0.25	0.25	12
	0.125	4.25	3.00	0.25	1.00	29
	0.25	3.29	2.71	0.14	0.43	18
	0.5	3.71	2.00	0.29	1.43	46
	1	4.00	0.00	1.00	3.00	100
	2	4.50	0.00	0.50	4.00	100
	5	4.50	0.00	0.00	4.50	100
10	0	4.75	4.00	0.75	0.00	16
	0.06	2.00	2.00	0.00	0.00	0
	0.125	3.00	3.00	0.00	0.00	0
	0.25	3.00	3.00	0.00	0.00	0
	0.5	4.00	2.40	0.20	1.40	40
	1	3.50	0.00	0.50	3.00	100
	2	4.75	0.00	0.25	4.50	100
	5	4.00	0.00	0.00	4.50	100

Table B-38 Effect of 0.5 mg PMA/kg of maternal bw on Microtus ochrogaster embryos when given at various days of gestation

Embryo age	Maternal dosage (mg/kg)	Average number of corpora lutea	Average number of live foetuses	Average number of preplacentation losses	Average number of postplacentation losses	Average pre- and postimplatation loss (% of litter)
7	0.5	4.75	2	0.25	2.25	58
8	0.5	3.8	1	0.40	2.40	74
9	0.5	3.71	2	0.29	1.43	46
10	0.5	4.0	2.4	0.2	1.40	40
11	0.5	4.0	3.5	0.00	0.50	13
12	0.5	3.5	3.5	0.00	0.00	0

Embryo-fetotoxic effect of some organic mercury compounds (Murakami, 1971)
Materials and methods: Seven days after vaginal plug was observed, 30 pregnant mice were administrated a small piece of vaginal contraceptive tablet in the vagina containing 0.1 mg PMA. In addition, twenty pregnant mice were given PMA sc.

Comments: Dose and experimental design for the mice given PMA sc was not described. Mice strain was not given. In general, this study is incomplete described.

Results: Increased embryonic deaths, slight changes of the spinal cord such as curvatures, etc. and malformations of the tail were detected. The incidence of embryonic deaths and abnormal progenies was statistical significance compared with the control animals. These results, however, were of those examined on day 14, and the final result at or near term.

Table B-39 Embryo effects of 0.1 mg PMA given pregnant mice seven days after vaginal plug

Results	Administration		
	Vaginal application	Subcutaneous injection	Control
No of treated animals	30	20	50
No of implants	212	137	332
Litter size	7.04	6.6	6.64
Normal progeny per litter	3.83	3.60	4.82
Foetuses without malformation:	115	66	243
-Normally developed	22	22	41
-Retarded in development			
Abnormal progenies:	15.1%**	9.15%**	2.7%
-Developed	19	7**	3
-Dead ones	13	5	6
Deaths during the embryonic stage:	20.3%**	24.2%**	11.8%
-Dead during day 10-12	1	0	3
-Dead before day 10	1	0	5
-Implantation sites and placental remnants	41	32	31

Results	Administration		
	Vaginal application	Subcutaneous injection	Control
Classification of malformations			
Exencephalia	1	1	0
Brain hernia	0	1	0
Microcephalic one (dead one)	1	1	0
Malformation of the eye (IBID)	1	1	0
Distenden C.N.S	1	0	3
Flexure or mal-closure of the spinal cord	16**	8	9
Abnormal tail	19**	4**	2
Blister formation	1	2*	0

*Statistically significant P<0.05
**Statistically significant P<0.01

Phenylmercury propionate
No data found.

Phenylmercury octanoate
No data found.

Phenylmercury neodecanoate
No data found.

Phenylmercury 2-ethylhexanoate
No data found.

B.5.9.2 Human information

No data found for any of the compounds.

B.5.9.3 Summary and discussion of reproductive toxicity

Phenylmercuric acetate

Exposure to 0.125 mg/kg bw PMA at day 8 in the gestation caused significantly increased implantation loss. The results also indicated that the toxic effect of PMA increased with increased dose and decreased embryo development. No maternal toxicity was observed in animals receiving a dose of 0.06 mg/kg bw. Taken together, the available data indicate that PMA cause adverse effect on reproduction.

Metabolites, degradation products and transformation products

According to UNEP (2002), studies of occupational exposure indicate that elemental mercury may affect human reproduction. In occupational exposure studies paternal exposure to metallic mercury does not appear to cause infertility or malformations, but pre-conception paternal urinary levels above 50µg/l are associated with a doubling of the spontaneous abortion risk (UNEP, 2002). Regarding reproductive toxicity elemental mercury is classified in EU as Repr. 1B; H360D - May damage the unborn child (CLP regulation, annex VI).

Several studies in animals have evaluated the possibility that developmental effects may occur after exposure to inorganic mercury salts. Based on these studies it can not be excluded that developmental effects may occur, but there are significant limitations to the studies that has been evaluated, according to UNEP (UNEP, 2008). Regarding fertility mercury dichloride and mercuric chloride are classified in EU as Repr. 2: H361f - Suspected of damaging fertility (CLP regulation, annex VI).

As regards the developmental effects of methylmercury the developing central nervous system is shown to be sensitive to methylmercury. Epidemiological studies have provided evidence that methylmercury in seafood consumed by pregnant women, even at mercury concentrations of 10-20% of those giving effects in adults, appears to have subtle, persistent effects on children's mental development as observed at the age of 4 to 7 (UNEP, 2008). Infants exposed to high levels of methylmercury during pregnancy may be born with cerebral palsy manifested by microcephaly, hyperreflexia, and gross motor and mental impairment, and some times blindness and deafness (UNEP, 2002): In milder cases, the effects may only be apparent later during the development as psychomotor and mental impairment and persistent pathological reflexes (UNEP, 2002). Effects on fertility following exposure to methylmercury are base on animal studies. It has been shown that, methylmercury at low doses may adversely affect reproduction in both males and females (UNEP, 2002). The former TC C&L group in exECB have concluded the following classification for methylmercury: Repr. Cat. 1, R61 – May cause harm to unborn child; Repr. Cat. 3, R62 – Possible risk of impaired fertility; R64 – May cause harm to breast-fed babies (ClassLab, Ex-ECB, 2010).

B.5.10 Other effects

B.5.10.1 Non-human information

B.5.10.1.1 Neurotoxicity

No data found for any of the phenylmercury compounds, except for some diffuse histopathological findings described by Swensson (1952). We question these findings, for more information see Section B.5.6.3.

Metabolites, degradation products and transformation products

Effects on the nervous system appear to be the most sensitive toxicological endpoint observed following exposure to elemental mercury. Accidental exposure to high concentrations of elemental mercury vapours, as well as, studies of populations/workers chronically exposed to potentially high concentrations of this vapour have shown effects on cognitive, sensory, personality and motor function (UNEP, 2002). One characteristic symptom after long-term high dose exposures (inhalation of concentrations above 0.5 mg/m3 for many years) is muscle tremors, which may progress to chronic spasm of the extremities (SCENIHR, 2008). It was concluded in a recent assessment of all studies on the exposure-response relationship between inhaled mercury and adverse health effects that several studies consistently demonstrate subtle effects on the central nervous system after long-term occupational exposure. These effects were observed at exposure levels of around 20 μg/m3 and higher (WHO 2003).

Few studies are available concerning neurological toxicity following oral exposure of humans to inorganic mercury (EPA, 1997). There are, however, several animal studies in which inorganic mercury induced-neurotoxicity have been reported (EPA, 1997).

The nervous system is the principal target tissue of methylmercury. In adults, the earliest effects of methylmercury poisoning are symptoms such as paresthesia, discomfort, and blurred vision. At higher exposure the following symptoms may appear; disturbances of the visual field, deafness, dysartheria, ataxia, and ultimately coma and death (UNEP, 2002). Effects on the central nervous system including ataxia and paresthesia have been observed in subjects with blood mercury levels as low as 200 μg Hg/l, corresponding to 50 μg Hg/g of hair (EPA, 1997).

B.5.10.1.2 Immunotoxicity

No data found for any of the phenylmercury compounds.

Metabolites, degradation products and transformation products

Available evidence suggests that the immune reaction to elemental mercury exposure is idiosyncratic; with either increases or decreases in immune activity depending on the genetic predisposition (EPA, 1997).

The most sensitive adverse effect observed following exposure to Hg2+ is the formation of autoimmune glomerulonephritis (inflammation of the kidney) (UNEP, 2008).

Methylmercury and ethylmercury are more potent immunosuppressors of the immune system than inorganic mercury and elemental mercury (SCENIHR, 2008).

B.5.11 Derivation of DNEL(s) /DMELs[4] or other quantitative or qualitative measure for dose response

The guidance on information requirements and chemical safety assessment, chapter R.8: "Characterisation of dose [concentration]-response for human health" has been applied to derive the DNELs (ECHA, 2008a).

So far no apparent threshold has been identified for neurotoxicity in children exposed to methylmercury in utero (Castoldi *et al*., 2008; Rice 2004). The threshold for neurological effects from mercury vapour has also been questioned recently (Richardson *et al*., 2009). The concept of DNEL or DMEL for mercury was introduced in this report in order to mention previous assessment works; however the chosen approach is a non-threshold approach.

DNEL for workers (long-term, inhalation, systemic effects)

Phenylmercury acetate
NOAEC
Results from a chronic two years oral rat study were used to derive a DNEL for PMA (Fitzhugh *et al*., 1950). The NOAEL in this study is based on renal damage which is the most sensitive endpoint for PMA exposure. The NOAEL was set at 0.0084 mg PMA/kg bw/day.
Exposure of workers is thought to be via inhalation. Guidance default values are applied for absorption (50 % via oral uptake and 100 % via inhalation). The NOAEL from the oral rat study is therefore converted into an inhalatory NOAEC for humans according to guidance on information requirements and chemical safety assessment chapter R.8. as follows:

Corrected inhalatory NOAEC = oral NOAEL * (1/0.38 m^3/kg bw/d^5) * (absorption (ABS) oral rat/ABS inhalation human) * 6.7m^3 (8h)/10m^3 (8h)

Corrected inhalatory NOAEC =
0.0084 mg/kg bw/d * 1/0.38 m^3/kg bw/d * (50%/100%) * 6.7/10
Corrected inhalatory NOAEC (8 h) = 0.0074 mg/m^3

DNEL
The assessment factors used in the extrapolation of experimental data into the human situation where as follow:
Interspecies differences (from rat to human): 1 (species differences in absorption rate and respiratory volume already accounted for in the calculation from oral NOAEL to inhalatory NOAEC. Additional allometric scaling factor not applied in accordance with Table R.8-4 in Guidance)
Intraspecies differences (workers): 5
Differences in duration of exposure: 1
Issues related to dose-response: 1
Quality of the whole database: 2 (the database is small, this factor could perhaps set be higher)
Total assessment factors (AF): 1*5*1*1*2 = 10

DNEL for workers (long-term, inhalation, systemic effects):

[4] This heading has been slightly modified compared to the format given in Annex I of the REACH regulation (section 7) to clarify the content of the section.
[5] Default standard respiratory volume for rats, as given in Table R.8-2 in Guidance

DNEL = NOAEC/AF = 0.0074 mg/m^3/10 = 0.00074 mg/m^3 = 0.74 µg/m^3

Elemental mercury
IPCS concluded that several studies consistently demonstrate subtle effects on the central nervous system in long-term occupational exposures to mercury vapour at exposure levels of approximately 20 µg/m3 or higher (WHO, 2003). This value is considered to be a LOAEC.

Assessment factors:
Interspecies differences: 1
Intraspecies differences (workers): 5
Dose-response relationships (starting point LOAEL): 3
Quality of the whole database: 1
Total assessment factors (AF): 1*5*3*1 = 15

Worker DNEL long-term for the inhalation route:
DNEL = LOAEC/AF = 20 µg/m^3/15 = 1.33 µg/m^3

Table B-40 DN(M)EL for workers

Exposure pattern	Compound	Route	Descriptors	DNEL/DMEL (appropriate unit)	Most sensitive endpoint
Long-term – systemic effects	Phenylmercury compound	Inhalation	DNEL	0.74 µg/m^3	Kidney damage
Long-term – systemic effects	Mercury vapour (elemental mercury)	Inhalation	DNEL	1.33 µg/m^3	Effects on the central nervous system

An indicative occupational exposure limit (IOEL) has been set for mercury at 0.02 mg/m3 (20 µg/m3) (Comission Directive 2009/161/EU). En ECHA guidance document indicates when IOELs can be applied by registrants (Appendix R.8.13, in ECHA 2010g). It was chosen not to apply the IOEL instead of the DNEL, since 20 µg/m3 is considered to be a LOAEC (WHO, 2003).

DNEL for the general population
Phenylmercury acetate
NOAEC
Results from a chronic two years oral rat study were used to derive a DNEL for PMA (Fitzhugh *et al*., 1950). The NOAEL in this study is based on renal damage which is the most sensitive endpoint for PMA exposure. The NOAEL was set at 0.0084 mg PMA/kg bw/day.
Exposure of the general population is thought to be via inhalation. Guidance default values are applied for absorption (50 % via oral uptake and 100 % via inhalation). The NOAEL from the oral rat study is therefore converted into an inhalatory NOAEC for humans according to guidance on information requirements and chemical safety assessment chapter R.8. as follows:

Corrected inhalatory NOAEC = oral NOAEL * (1/1.15 m^3/kg bw/d^6) * (absorption (ABS) oral rat/ABS inhalation human)
Corrected inhalatory NOAEC = 0.0084 mg/kg bw/d * 1/1.15 m^3/kg bw/d * (50%/100%)
Corrected inhalatory NOAEC (24 h) = 0.00365 mg/m^3

The assessment factors used in the extrapolation of experimental data into the human situation where as follow:
Interspecies differences (from rat to human): 1 (species differences in absorption rate and respiratory volume already accounted for in the calculation from oral NOAEL to inhalatory NOAEC. Additional allometric scaling factor not applied in accordance with Table R.8-4 in Guidance)
Intraspecies differences (general public): 10
Differences in duration of exposure: 1
Issues related to dose-response: 1
Quality of the whole database: 2 (the database is small, this factor could perhaps set be higher)
Total assessment factors (AF): 1*10*1*1*2 = 20

General-population DNEL long-term for the inhalation route:
DNEL = NOAEC/AF = 0.00365/20 =0.000183 mg/m^3 = 0.18 µg/m^3

Phenylmercury propionate
No data.

Phenylmercury octanoate
No data.

Phenylmercury neodecanoate
No data.

Phenylmercury 2-ethylhexanoate
No data.

Elemental mercury
In 2003 the International Programme on Chemical Safety (IPCS) evaluated all available studies on the exposure-response relationship between inhaled mercury vapour and adverse health effects. IPCS concluded that several studies consistently demonstrate subtle effects on the central nervous system in long-term occupational exposures to mercury vapour at exposure levels of approximately 20 µg/m^3 or higher (WHO, 2003). To derive a LOAEL for the general population the IPCS further calculated that an extrapolation from a 8 hours/day, 40 hours/work week exposure to a continuous 24 hours/day, 7 days/week (8/24 and 5/7) would give an equivalent of 4.8 µg/m^3. This value is considered to be a LOAEC. The Norwegian Institute of Public Health used the LOAEC of 4.8 µg/m^3 estimated by IPCS as the dose descriptor to derive a DNEL for the general population following the guidance on information requirements and chemical safety assessment chapter R.8:

The assessment factors used were as follows:
Intraspecies differences (general population):10

[6] Default standard respiratory volume for rats, as given in Table R.8-2 in Guidance

Dose-response relationships (starting point LOAEL): 3
Quality of the whole database: 1
Total assessment factors (AF): 10*3*1 = 30

General-population DNEL long-term for the inhalation route:
DNEL = LOAEC/AF = 4.8/30 = 0.16 µg/m^3

The DNEL derived for the general population is in the same range as the estimated tolerable concentration of 0.2 µg/m^3 derived by IPCS for the general population long-term inhalation exposure to elemental mercury vapour. The US ATSDR established a minimum risk level (MRL) of 0.2 µg/m^3 for metallic mercury, also based on the occupational data (ATSDR, 1999). The EPA has derived a reference concentration (RfC) of 0.3 µg/m^3 for exposure of the general population to elemental mercury vapour (EPA 1997).

Methylmercury
The Joint FAO/WHO Expert Committee on Food Additives (JECFA) established a Provisional Tolerable Weekly Intake (PTWI) of 1.6 µg/kg bw/week for methylmercury. The Committee based the PTWI on the evaluation on studies from the Faroe Islands and Seychelles Island and used the average of the estimated maternal hair concentration associated with no-observed–effect-level/benchmark dose level (NOEL/BMDL) for neurotoxicity associated with in utero exposure. The Committee determined that a steady-state daily ingestion of methylmercury of 1.5 µg/kg bw/day would result in concentrations in maternal blood estimated to be without appreciable adverse effects in the offspring in the Faroe and Seychelles Island studies. In 2006, JECFA confirmed that the PTWI of 1.6 µg/kg bw/week remained appropriate for protection of the most vulnerable life stages, the embryo and foetus (FAO/WHO, 2007). A DNEL for methylmercury was determined based on the NOEL/BMDL of 1.5 µg/kg bw/day.

The assessment factors used were as follow:
Intraspecies differences (general public):10
Quality of the whole database: 1
Total assessment factors (AF): 10*1 = 10

General-population DNEL long-term for the oral route:
DNEL = LOAEL/AF = 1.5/10 = 0.15 µg/kg bw/day

This DNEL correlates well with the PTWI derived by the IPCS which if extrapolated to daily intake would correspond to 0.23 µg/kg bw/day (1.6/7). EPA derived a reference dose (RfD) of 0.1 µg/kg bw/day based the studies from Faroe Islands and Seychelles Island and a smaller study from New Zealand (EPA, 2001).

Overview of typical dose descriptors for all endpoints

Table B-41 DN(M)ELs for the general population[7]

Exposure pattern	Compound	Route	Descriptors	DNEL/DMEL (appropriate unit)	Most sensitive endpoint
Long-term - systemic effects	PMA	Inhalation (µg/m^3)	DNEL	0.18 µg/m^3	Kidney damage
	Elemental mercury	Inhalation (µg/m^3)	DNEL	0.16 µg/m^3	Effects on the central nervous system
	Methylmercury	Oral (µg/kg bw/day)	DNEL	0.15 µg/kg bw/day	Developmental neurotoxicity

[7] General population includes consumers and humans via the environment. In rare cases it may also be relevant to derive a DNEL for specific subpopulations, such as children. In this case the table need to be repeated. In addition as the respiration rate is taken into account for the derivation of the DNEL, this table need to be repeated in case different exposure scenarios lead to different respiration rate.

B.6 Human health hazard assessment of physico-chemical properties

B.6.1 Explosivity

No data is found, so it is not known if the 5 phenylmercury substances have explosive properties. None of them has been classified for this effect in the CLP regulation.

B.6.2 Flammability

No data is found, so it is not known if the 5 phenylmercury substances have flammable properties. None of them has been classified for this effect in the CLP regulation.

B.6.3 Oxidising properties

No data is found, so it is not known if the 5 phenylmercury substances have oxidising properties. None of them has been classified for this effect in the CLP regulation.

B.7 Environmental hazard assessment

The environmental effects of phenylmercury acetate, phenylmercury 2-ethylhexanoate, phenylmercury propionate, phenylmercury octanoate and phenylmercury neodecanoate have been assessed. However, the ecotoxicity data available for these five compounds are limited. Furthermore, where there is information on these phenylmercuric compounds, the quality of the corresponding study is not satisfactory in many cases. Moreover, phenylmercury compounds are degraded in the environment to give hazardous degradation products, i.e. inorganic mercury and elemental mercury, which can be transformed to methylmercury. Therefore, the hazard assessment of phenylmercury compounds has been extended to include other forms of mercury including among others ethylmercury, dimethylmercury, methylmercury and ionic mercury.

The risks that might arise from the degradation/transformation products of phenylmercury compounds have been assessed as well. PNEC's for those degradation/transformation products have been derived and a quantitative risk assessment is presented in Appendix 1.

B.7.1 Aquatic compartment (including sediment)

B.7.1.1 Toxicity data

B.7.1.1.1 Fish

B.7.1.1.1.1 Short-term toxicity to fish

Phenylmercury acetate
Joshi and Rege (1980) studied the acute toxicity of phenylmercury acetate (PMA) on female mosquito fish (*Gambusia affinis*). The authors reported general water quality parameters for the study that was conducted, but not the concentration ranges that were tested or if they had a proper control group. In addition, only some of the LC50 values reported 95 % confidence intervals. LC_{50} values for fish, exposed to PMA for 24, 48, 72, and 96 hours were 115, 72, 56, and 37 µg/L Hg, respectively. These values were 5-8 times lower than the corresponding LC_{50} values they reported for mercuric chloride. The 96 hour LC_{50} from this study was 37 µg/L and the Klimisch score for this study is considered to be 3 (not reliable, based on lack of chemical analysis, statistics and a lack of a control group).

Kihlström and Hulth (1972) studied the effect of PMA on the hatching of eggs from zebrafish (*Danio rerio*). Eggs were fertilized in clean water and transferred to solutions containing nominal concentrations of 6, 12, and 30 µg/L PMA. No eggs hatched at the highest concentration. Significantly more eggs hatched at the lowest concentration compared with the control group plus they hatched sooner than the control eggs. However it is unclear whether this is due to PMA or some other abiotic variable such as culture conditions. The number of eggs hatched in the solution containing 12 µg/L PMA was not significantly different from the control, but they also hatched earlier. Therefore, the LOEC for this study was 30 µg/L and the NOEC was 12 µg/L. The Klimisch score for this study is considered to be 2 (reliable with restrictions based on the lack of confirmatory chemical analysis).

Matida *et al*. (1971) studied the acute toxicity of waterborne and dietary PMA, methylmercury chloride, ethylmercury phosphate, and mercury chloride to rainbow trout (*Oncorhynchus mykiss*) fingerlings in a semi static procedure. They didn't report the concentration ranges that were tested, or the numbers of fish that were used. LC_{50} values were however reported and for PMA they were calculated to be 19 µg/L (12 h), 15 µg/L (24 h), 11 µg/L (48 h), 11 µg/L (72 h), and 8.6 µg/L (96 h). These were about 3.5, 6, and 15 times lower than the corresponding values for methylmercury chloride, ethylmercury phosphate, and mercury chloride, respectively indicating that PMA is more toxic than the other mercuric compounds that were tested. The Klimisch score for this study is considered to be 2 (reliable with restrictions based on the lack of chemical analysis and insufficient data).

In summary, the data from Matida *et al*. (1971) indicated that the acute toxicity of PMA to Rainbow trout fingerlings was at a concentration of 8.6 µg/L. This is the most sensitive endpoint using the most sensitive life stage in the evaluation of short term toxicity to fish.

Table B-42 Short term toxicity to fish

Method	Results	Remarks	Reference
Acute toxicity of PMA to female mosquito fish (*Gambusia affinis*)	LC_{50} values for PMA at 24, 48, 72, and 96 hours were 115, 72, 56, and 37 µg/L Hg, respectively	No indication of concentration ranges that were tested, or if a control was used. Only some of the LC_{50} values reported a 95 % confidence interval	Joshi and Rege (1980)
The effect of PMA on the hatching of zebrafish (*Danio rerio*) eggs	No eggs hatched at the highest concentration of 30 µg/L	Eggs were exposed to nominal concentrations of 6, 12, and 30 µg/L PMA	Kihlström and Hulth (1972)
Toxicity of PMA to rainbow trout (*Oncorhynchus mykiss*) fingerlings	LC_{50}s of PMA were 19 µg/L (12 h), 15 µg/L (24 h), 11 µg/L (48 h), 11 µg/L (72 h) and 8.6 µg/L (96 h)	Concentration ranges tested and number of fish used was not reported, solutions were renewed daily	Matida *et al*. (1971)

Phenylmercury propionate, -octanoate, 2-ethylhexanoate and -neodecanoate
No data found.

Other Mercury compounds
The dominant form of mercury found in fish is methylmercury which can account for more than 95% of the total body burden (Bloom, 1992). Therefore, factors affecting methylation are of principle importance in evaluating the risk and hazards of mercury in fish. According to the UNEP Global mercury assessment report, the effects of mercury at higher levels of biological organisation such as ecosystem, community and population are not well understood. However there have been numerous papers that have been published on the ecotoxicity of mercury *per se*. Interestingly, the UNEP report suggests that exposure to waterborne methylmercury is not of serious concern to adult fish but may be more important when considering indirect exposure via dietary exposure or maternal transfer. For example, Hg levels affecting embryos via maternal transfer can be two orders of magnitude lower concentrations than those

affecting adult fish. The UNEP report further indicates that acute toxicity to freshwater fish can be within the ranges of 33-400 µg/L while seawater fish are less sensitive to mercury.

In relation to methylmercury, Birge *et al*. (1983) determined the acute toxicity to rainbow trout embryos exposed for 4 days post hatch. The results for acute toxicity (LC50) were 5 µg/L after 4 days exposure. This indicates that the acute toxicity for methylmercury was consistent with the most sensitive endpoint for PMA. With regards to methylmercuric chloride, Matida *et al* (1971) determined that the 96 hour LC_{50} to rainbow trout fingerlings was 31 µg/L.

B.7.1.1.1.2 Long-term toxicity to fish

Phenylmercury acetate

There are very limited data available for long term toxicity tests with fish to PMA, however in one experiment by Matida *et al*. (1971), they exposed rainbow trout fingerlings to water containing 0.11 and 1.1 µg/L PMA for 12 weeks in a flow-through experiment. There were no mortalities, but growth appeared to be retarded in the higher concentration of 1.1 µg/L PMA, resulting in a LOEC of 1.1 µg/L PMA and a NOEC of 0.1 µg/L PMA. However, there were no statistical analyses to confirm these results. Furthermore, there were no control groups used to compare the growth rates. In another experiment of the same study rainbow trout fingerlings were fed for 28 weeks with commercial trout feed spiked with PMA or ethylmercury phosphate to a Hg concentration of 5 ppm (Matida *et al*., 1971). Fish fed the exposed feed exhibited an apparent decrease in growth and there appeared to be no effect on survivorship. The Klimisch score for this study is considered to be 3 (not reliable based on the lack of proper experimental design, no control organisms and no statistical comparisons).

In summary, the findings of Matida *et al*. (1971) was the study with the most sensitive endpoint (LOEC and NOEC of 1.1 and 0.1 µg/L respectively) in relation to all the studies that were assessed for both acute and chronic endpoints. However there are insufficient data to indicate if there is a statistically significant difference from a control, and therefore due to the uncertainty of the data, it will be not used for the derivation of the PNEC in freshwater.

Table B-43 Long- term toxicity to fish

Method	Results	Remarks	Reference
Toxicity of PMA to Rainbow trout fingerlings	No mortalities but growth was recorded to be retarded in the (LOEC) **1.1 µg/L** concentration after 12 weeks	Concentrations tested were 0.11 and 1.1 µg/L PMA	Matida *et al*. (1971)
Rainbow trout fingerlings toxicity to PMA methylmercury, mercury chloride and ethylmercury phosphate	Decrease in growth, but no mortality observed.	Fish were fed for 28 weeks with exposed commercial trout feed	Matida *et al*. (1971)

Phenylmercury propionate, -octanoate, 2-ethylhexanoate and -neodecanoate
No data found.

Other mercury compounds
In the RPA report (2002) several studies on the toxicity of methylmercury are mentioned but not described in detail. In a study performed by Christensen *et al*. (1975) a 248 day growth test on larvae of brook trout (*Salvelinus fontinalis*). The NOEC was determined to be 0.08 µg/L. In a 48 day embryo mortality assessment of methylmercury to coho salmon (*Oncorhynchus kisutch*) the NOEC was reported to be 29 µg/L (Devlin and Mottet, 1992).

B.7.1.1.2 Aquatic invertebrates

B.7.1.1.2.1 Short-term toxicity to aquatic invertebrates

Crustaceans

Phenylmercury acetate
Krishnaja *et al*. (1987) studied the toxic effects of certain heavy metals on the intertidal crab (*Scylla serrata*). Acute toxicity was tested in semi static experiment (24 h renewal) using artificial sea water as the dilution water. Concentrations were not verified and 10 animals were used in each group plus an appropriate control. The LC_{50} values reported for Hg in the form of PMA were 700 µg/L (24 h), 580 µg/L (48 h) and 540 µg/L (96 h). The highest non-lethal concentration (NOEC) was 320 µg/L (96 h), while the lowest concentration causing 100 % mortality (LC_{100}) was 750 µg/L (96 h). The Klimisch score for this study is considered to be 3 (based on lack of analytical chemistry for verification of the test concentrations, and inappropriate test organism used).

Table B-44 Short-term toxicity to aquatic invertebrates

Method	Results	Remarks	Reference
Acute toxicity of PMA to the intertidal crab (*Scylla serrata*).	**LC50** values for PMA were 700 µg/L (24 h), 580 µg/L (48 h) and **540 µg/L** (96 h). (NOEC) was 320 µg/L (96 h), while the lowest concentration causing 100 % mortality (LC100) was 750 µg/L (96 h)	Semi static experiment (24h renewal) concentrations were not verified	Krishnaja *et al*. (1987)

Phenylmercury propionate, -octanoate, 2-ethylhexanoate and -neodecanoate
No data found.

Other mercury compounds
There is limited data available for acute/short term toxicity effects in crustaceans. The United Nations Environment Programme (UNEP) Global Mercury Assessment report (2002) indicates that larval stages of crustaceans can typically be 100 times more sensitive to mercury than the adult life stages. For example, EC_{50} values for larval stages may typically be

seen at concentrations of 10 µg/L, however the UNEP report (2002) does not give any further indication of species used or test type.

B.7.1.1.2.2 Long-term toxicity to aquatic invertebrates

Phenylmercury acetate

A long-term toxicity test (30 days) was conducted by Krishnaja *et al*. (1987) who studied the long term effects of certain heavy metals on the intertidal crab (*Scylla serrata*). Similar to the acute toxicity test above, the test was performed using a semi static experiment (24 h renewal) with artificial sea water as the dilution water. Concentrations were not verified and 10 animals were used in each group plus an appropriate control. Concentrations of Hg in the form of PMA tested were 320, 270, and 180 µg/L, but the exposure to the highest concentration was aborted after 17 days due to high mortality (>50 %). Both acute and long-term exposures were found to produce conspicuous histopathological changes in the hepatopancreas and gills. The Klimisch score for this study is considered to be 3 (based on lack of analytical chemistry for verification of the test concentrations, and inappropriate test organism used).

Biesinger *et al*. (1982) tested the chronic toxicity of methylmercury chloride, mercury chloride, and PMA to *Daphnia magna* under semi static conditions with the solutions renewed once a week. Four replicate test chambers with a total of 20 animals were used for each experimental treatment plus an appropriate control. Concentrations were verified by measurement of total concentrations of Hg and loss of mercury in solution was attributed to loss through adsorption to glassware, volatilization, and uptake by the organisms. Any effects on the animals were statistically analysed using analysis of variance (ANOVA). Concentrations (nominal/measured) of PMA tested were 0.63/0.35, 1.25/0.54, 2.50/1.12, 5.00/1.90 and 10.00/3.20 µg/L. The lowest (measured) concentrations (LOEC) of PMA found to significantly affect survival after 21 days of exposure was 1.90 µg Hg/L while the LOEC for production of young was 3.20µg Hg/L. The highest concentrations found to not cause any significant effect (NOEC) was 1.12 µg Hg/L and 1.90 µg Hg/L for survival and production of young, respectively. These data, although not generated according to test methods detailed in a specific test guideline (e.g. OECD 211), do appear robust. For example, there is an indication of the statistical approaches that were employed, the concentrations of PMA in the solutions are based on measured data and not nominal test data and there was an appropriate control group that was used. Based on this evaluation, the Klimisch criteria for this study should be 1. Furthermore, due to the assessed reliability of the data and considering the sensitivity of the endpoints, these data will be used for the derivation of the PNEC.

Table B-45 Long-term toxicity to aquatic invertebrates

Method	Results	Remarks	Reference
Chronic toxicity of PMA on the intertidal crab (*Scylla serrata*).	Concentrations of PMA tested were 320, 270, and 180 µg/L, highest concentration was stopped after 17 days due to high mortality (>50 %). Long-term exposures were found to produce conspicuous histopathological changes in the hepatopancreas and gills	Semi static experiment, exposure was 30 days in duration, concentrations were not verified	Krishnaja *et al*. (1987)
Chronic toxicity of PMA to *Daphnia magna*	The **NOEC** and LOEC of PMA found to significantly affect survival and reproduction after 21 days of exposure were **1.12** µg Hg/L and **1.90** µg Hg/L and 1.90 µg Hg/L and 3.20 µg Hg/L respectively	Semi static conditions, concentrations were based on measured data	Biesinger *et al*. (1982)

Other mercury compounds

The effect of methylmercury chloride and mercuric chloride on the survival and reproduction of *Daphnia magna* in a flow through system was also assessed by Biesinger *et al*. (1982). The LOEC/NOEC for methylmercury chloride was >0.26/0.26 µg Hg /L (survival) and 0.04/<0.04 µg Hg /L (production of young), while for mercuric chloride effects on survival and reproduction (LOEC/NOEC) was 2.70/1.28 µg Hg /L and 1.28/0.72 µg Hg /L respectively.

According to the RPA-report (2002), the most sensitive NOEC value for crustaceans and other invertebrates exposed to inorganic mercury is 0.07 µg/L, however due to the range of values reported, a geometric mean of 0.7 µg/L is recommended. There is however limited information in the RPA-report (2002) to describe details regarding test design and limitations of these results. Furthermore, this report also indicates that the most sensitive species to methylmercury is the tubellarian flatworm *Dugesia dorotocephala* with a NOEC value of 0.03 µg/L on fissioning and neurotoxic effects after 14 d exposure (Best *et al* 1981). The most sensitive NOEC endpoint on reproduction and growth for *Daphnia pulex* was 0.1 µg/L after 30 d exposure (Tian-yi & McNaught, 1992). However these NOEC values will not be used for the toxicity assessment of methylmercury due to the limited information on the test design.

B.7.1.1.3 3 Algae and aquatic plants

Phenylmercury acetate

Delcourt and Mestre (1978) studied the effect of PMA on the growth of the phytoplankton species *Chlamydomonas variabilis*. The concentrations tested were 0.2, 0.5, 1.0, 1.5, 2.0, 5.0, and 15 µg/L Hg as PMA (nominal concentrations). Growth in the concentrations less than 1 µg/L was not significantly different from the control. The growth of algae exposed to the higher concentrations had a lag phase before the exponential growth phase which was proportional to the concentration of PMA. The duration of the exponential phase also decreased for concentrations higher than 1 µg/L. However, PMA did not affect the final concentration of cells, only the time necessary to reach the threshold (up to 18 days). The

Klimisch score for this study is considered to be 3 (based on insufficient data regarding the study and no analytical chemistry for verification of the test concentrations).

Harris *et al*. (1970) exposed a marine diatom (*Nitzschia delicatissima*) to 1, 10, and 50 µg/L of Hg (single application) as either PMA, diphenylmercury, or methylmercury. The effects on photosynthesis (uptake of radiolabelled carbon) and growth were assessed. The toxicant was added to the marine diatom when population was in the exponential phase of growth. After 24 hours of exposure, radiolabelled sodium bicarbonate was added and test bottles were returned to a growth chamber for 5 hours exposure to light before the samples were filtered and the radioactivity measured. Effects of mercurials on photosynthesis and growth were calculated by dividing the net count at each concentration by the net count of the control sample. Significantly lower counts relative to the control were observed at 1 µg/L Hg as PMA and 10 µg/L of Hg as diphenylmercury. At 50 µg/L of Hg as PMA all uptake of inorganic carbon had stopped and cell counts indicated complete inhibition of growth.

A similar test using the same concentrations of mercurials was conducted with a natural phytoplankton community. Samples from the natural communities were taken after 24, 72 and 120 hours. Radiolabelled sodium bicarbonate was added and after 5 hours of light exposure the effect on photosynthesis and growth was assessed as described above. Significantly decreased counts relative to the control were observed after exposure to 1 µg/L Hg as PMA or diphenylmercury. The Klimisch score for this study is considered to be 3 (based on relevant study design and no analytical chemistry for verification of the test concentrations).

Table B-46 Toxicity to Algae and aquatic plants

Method	Results	Remarks	Reference
Effect of PMA on the growth of the phytoplankton species *Chlamydomonas variabilis*	Growth affected in concentrations ≥1 µg/L Hg as PMA	Concentrations tested were 0.2, 0.5, 1.0, 1.5, 2.0, 5.0, and 15 µg/L Hg as PMA (nominal concentrations). Effects by a lag phase before the exponential growth phase	Delcourt and Mestre (1978)
Effect of PMA on photosynthesis, uptake of radiolabelled carbon and growth to a marine diatom (*Nitzschia delicatissima*)	Significantly lower counts relative to control observed at 1 µg/L Hg as PMA. At 50 µg/L Hg as PMA all uptake of inorganic carbon had stopped and there was complete inhibition of growth. A similar test with a natural phytoplankton community revealed significantly decreased counts relative to the control after exposure to 1 µg/L Hg as PMA	Concentrations of 1, 10, and 50 Hg as PMA µg/L. Effects on photosynthesis and growth	Harris *et al*. (1970)

Phenylmercury propionate, -octanoate, 2-ethylhexanoate and -neodecanoate
No data found.

Other mercury compounds
According to the RPA report (2002) a study on the toxicity of inorganic mercury to the blue green alga *Microcystis aeruginosa* indicated a threshold toxicity value of 5 µg/L and a NOEC value of 2.5 µg/L.

In addition, the authors of the RPA report (2002) indicated that there is very little or no toxicity data for methylmercury in the published literature so data on a marine macrophyte oarweed (*Laminaria saccharina*) was recommended to be used. A NOEC of 1 µg/L on development of zoospores and growth of sporophytes after 14 d exposure was determined (Thompson & Burrows, 1984).

The effect of diphenylmercury, on photosynthesis, uptake of radiolabelled carbon and growth to a marine diatom (*Nitzschia delicatissima*) were reported by Harris *et al*. (1970). Significantly lower radioactive counts relative to the control were observed at 10 µg/L of Hg as diphenylmercury. The details of this study are insufficiently detailed and no further information could be obtained from these results.

B.7.1.1.4 Sediment organisms

Phenylmercury acetate, propionate, -octanoate, 2-ethylhexanoate and -neodecanoate
No data found.

Other mercury compounds
According to the RPA report (2002) the amphipod *Hyalella azteca* was exposed to inorganic mercury and the resulting NOEC was 0.62 µg/L. However the data pertaining to this study is limited and no other data on sediment dwelling organisms was found.

B.7.1.1.5 Other aquatic organisms

Bivalves

Phenylmercury acetate
Kopfler (1974) exposed eastern oyster (*Crassostrea virginica*) to PMA in a flow-through experiment where the organisms were exposed throughout the experiment. Concentrations of PMA in the test solutions were verified by measuring PMA as total Hg present in the water. In the first experiment, a concentration of 50 µg/L PMA (as Hg) was used at a test temperature between 0-10ºC. In the second experiment a concentration of 1 µg/L and a test temperature of 25-35 ºC was used. The first experiment was terminated after 19 days because many of the oysters exposed to PMA died or became moribund (e.g. slow or incomplete valve closure when disturbed). The surviving oysters in these groups were placed in clean water, but they all died within 14 days. High mortality also occurred in the second experiment for oysters exposed to PMA over 74 days. Oysters exposed to PMA accumulated Hg to a

concentration of about 100 ppm wet weight and this was consistent with the quantity of Hg that was accumulated in oysters exposed to methylmercury. This indicates that PMA (measured as Hg) accumulates in the tissue of oysters to the same degree as methylmercury. However, since PMA was only measured as Hg and not as the parent compound, it is not possible to determine if the Hg which had accumulated in the tissue was PMA or a metabolic product. The Klimisch score for this study is considered to be 3 (not reliable, based on the lack of chemical analysis, test organism and insufficient data).

Watling and Watling (1982) studied the effect of PMA on the filtering rate of the Brown mussel (*Perna perna*). The mussels were exposed for 1 hour, and the solutions were apparently determined to be stable for the one-hour period required for each experiment. However, the range of concentrations tested was not reported so it is unclear if the concentrations of Hg were actually measured. The concentration found to cause a 50 % reduction in filtering rates were 20µg/L. The Klimisch score for this study is considered to be 3 (based on: not a relevant study design, insufficient details regarding the studies and no analytical chemistry for verification of the test concentrations).

Table B-47 Toxicity to bivalves

Method	Results	Remarks	Reference
Uptake of PMA into Eastern oyster (*Crassostrea virginica*)	1st experiment terminated because of dead or moribund oysters. High mortality also occurred in the 2nd experiment but this was over a longer duration (74 days). Oysters had accumulated PMA to a concentration of about 100 ppm wet weight	A concentration of 50 µg/L used in the first experiment. The second experiment used a concentration of 1 µg/L	Kopfler (1974)
Effect of PMA on the filtering rate of the Brown mussel (*Perna perna*)	A concentration of 20 µg/L was found to cause a 50 % reduction in filtering rates in the mussels	Mussels exposed for 1 hour, conc-entration range not reported	Watling and Watling (1982)

Phenylmercury propionate, -octanoate, 2-ethylhexanoate and -neodecanoate
No data found.

Other mercury compounds
Kopfler (1974) exposed eastern oyster (Crassostrea virginica) to waterborne Hg in the form of methylmercury chloride, and mercuric chloride in a flow-through experiment. Aqueous concentrations were verified by measurements of Hg. A concentration of 50 µg/L Hg was used in the first experiment at a test temperature between 0-10ºC. As with the results from the PMA experiments in the same study by Kopfler (1974), the experiment was terminated after 19 days because many of the oysters receiving methylmercury were dead or moribund (slow, incomplete valve closure when disturbed). Again, the surviving oysters in these groups were placed in clean water, but they all died within 14 days. Oysters exposed to mercuric chloride suffered no apparent ill effects over a 42-day exposure period. In a second experiment a concentration of 1 µg/L and a test temperature of 25-35 ºC were used. High mortality also occurred in this experiment for oysters receiving methylmercury over 74 days.

Watling and Watling (1982) studied the effect of waterborne exposure of ethylmercury chloride, methylmercury chloride and mercury chloride, on the filtering rate of the Brown mussel (*Perna perna*). The mussels were exposed for 1 hour, and the solutions were indicated to be stable for the one-hour period required for each experiment. However, the range of concentrations tested was not reported so it is unclear if the concentrations of Hg were actually measured. Concentrations found to cause a 50 % reduction in filtering rates were 30, 50, and 25 µg/L for Hg in the forms of ethylmercury chloride, methylmercury chloride and mercuric chloride, respectively.

B.7.1.2 Summary of effects

Data selected on the most relevant endpoints for both acute and chronic toxicity to phenylmercury acetate

Phenylmercury acetate

Table B-48 Summary of effects for PMA

	Species	Value	Remarks/Justification
Acute toxicity	Mosquito fish (*Gambusia affinis*)	37 µg/L	96 h LC_{50} (Joshi and Rege ,1980)
	Zebrafish (*Danio rerio*)	30 µg/L	LOEC non hatching of eggs (Kihlström and Hulth, 1972)
	Rainbow trout fingerlings (*Onchorynchus mykiss*)	8.6 µg/L	96 h LC_{50} (Matida *et al*., 1971)
	Intertidal crab (marine) (*Scylla serrata*)	540 µg/L	96 h LC_{50} (Krishnaja *et al*., 1987)
	Algae (*Chlamydomonas variabilis*)	>1 µg/L	Growth affected by a lag phase before the exponential growth phase (Delcourt and Mestre, 1978)
	Brown mussel (marine) (*Perna perna*)	20 µg/L	50% reduction in filtering rate (Watling and Watling, 1982)
Chronic toxicity	Rainbow trout (*Onchorynchus mykiss*)	1.1/0.11 µg/L	12 weeks LOEC/NOEC on growth (Matida *et al*., 1971)
	Intertidal crab (marine) (*Scylla serrata*)	<180 µg/L	30 days NOEC (Krishnaja *et al*., 1987)
	Water flea (*Daphnia magna*)	1.90/1.12 µg Hg/L	21 days LOEC/NOEC survival (Biesinger *et al*., 1982)

Phenylmercury propionate, -octanoate, 2-ethylhexanoate and -neodecanoate

No data found.

Methylmercury

Data selected on the most relevant endpoints for both acute and chronic toxicity to methylmercury

Table B-49 Summary of effects for methylmercury

	Species	Value	Remarks/Justification
Acute toxicity (methylmercury)	Rainbow trout *(Onchorynchus mykiss)*	5.0 µg/L	96 h LC_{50} (Birge *et al*. 1983)
Chronic toxicity (methylmercury)	Brook trout (*Salvelinus fontinalis*)	0.08 µg/L	248d NOEC based on growth of larvae. Christensen *et al*. (1975)
Chronic toxicity (methyl mercuric chloride)	Water flea (*Daphnia magna*)	>0.26/0.26 µg Hg /L (survival)	LOEC/NOEC survival (Biesinger *et al*., 1982)
Chronic toxicity (methylmercury)	Tubellarian flatworm (*Dugesia dorotocephala*)	0.03 µg/L	14 d NOEC based on fissioning and neurotoxic effects (Best *et al*. 1981)
Aquatic Plants (methylmercury)	Marine macrophyte, Oarweed (*Laminaria saccharina*)	1 µg/L	14 d NOEC on development of zoospores, growth of sporophytes (Thompson & Burrows, 1984)

B.7.1.3 PNEC water

Predicted no-effect concentrations (PNECs) have been generated. Due to lack of data and also due to the fate of phenylmercury compounds in the environment it is proposed to perform the quantitative risk assessment for environment on the basis of the inorganic mercury data. As the estimation of PEC-values is afflicted with great uncertainty, this dossier relies predominantly on the PBT-like properties of the degradation/transformation product methylmercury. The calculation of PNEC-values as part of the quantitative risk assessment is presented in Appendix 1.

B.7.2 Terrestrial compartment

The phenylmercury compounds are degraded to hazardous degradation products, i.e. inorganic mercury compounds and elemental mercury, which can be transformed to methylmercury. Risks that might arise from these degradation/transformation products have been assessed as well. PNEC's for those degradation/transformation products have been derived and a quantitative risk assessment is presented in Appendix 1.

B.7.2.1 Toxicity data

Mercury in soil exists in many forms, including elemental mercury (Hg^0), ionic mercury (Hg II), methylmercury (MeHg), mercury hydroxide ($Hg(OH)_2$), and mercury sulfide (HgS). Inorganic mercury (Hg (II)) is the predominant toxic form of mercury in soils (Heaton *et al*., 2005).

The toxicity of inorganic and organomercuric compounds is based on their interaction with sulphydryl groups of enzymes (Fent, 2003). Furthermore, mercury competes with essential elements as zinc and calcium. The toxic effects of mercury depend on its chemical form and the route of exposure. As discussed previously, organomercury compounds are highly toxic to all organisms. Methylmercury is the most toxic mercury compound due to its stability and high lipophilicity. Elemental and inorganic mercury are less toxic to terrestrial organisms than methylmercury (Stein *et al*., 1996).

Inorganic mercury (Hg^{2+}) can change into the organic form by soil bacteria (Fukunaga *et al*., 1972, Tonomura *et al*., 1972). In aquatic sediments the formation from Hg (II) to methylmercury is of greater concern than in soil. Monomethylmercury formation is favoured under acidic conditions in soils. Dimethylmercury is favoured under neutral or alkaline conditions in the presence of a strong complexing agent (Stein *et al*., 1996). The amount of methylmercury in soils is low relative to total mercury. According to Boudou and Ribeyre (1997), the normal percentage of total mercury in the form of methylmercury in soils ranges between 0.5 and 1.5%. Organic mercury compounds are efficiently taken up by biological systems and their accumulative properties are high (Haney and Lipsey, 1973, Hukabee and Blaylock, 1973, Nuorteva *et al*., 1980). The typical global mercury content of soils ranges between 0.03 and 0.15 mg kg^{-1} dry weight (Floyd *et al*., 2002).

Soil parameters like pH and the content of organic matter influence the bioavailability of chemicals. Most important is the dissolved concentration of a chemical in the pore water. In soils, mercury is mainly bound to higher molecular weight substances. In acidic soils, more mercury is released than in neutral and basic soils. High amounts of organic matter reduce the release of mercury. Thus, the highest release of mercury either by volatilization or by leaching occurs in acidic soils containing little organic matter.

Microbial activation is evident in the methylation of inorganic mercury in aquatic sediments and other environments to yield the more toxic mono- or dimethylmercury-compounds that are harmful (Alexander, 1981). The production of methylmercury is much higher in aquatic sediments than in soil because it is mostly formed at anoxic conditions by sulfate and iron-reducing bacteria. Holloway *et al*. (2009) found that the formation of methylmercury appears to be most strongly linked to soil moisture. Furthermore, the soil moisture content was directly related to the content of phospholipid fatty acids biomass in wetland soils. The

greatest concentrations of methylmercury were measured in wetland soils and soil of volcanic origin. Mercury methylation was associated with sulfate-reducing bacteria, including *Desulfobacter sp*. and *Desulfovibrio sp*., although these organisms were not exclusively responsible for Hg methylation.

Phenylmercury acetate

There are only few data available on how phenylmercury acetate affects terrestrial organisms. Little is known about the effects of its metabolites. Phenylmercury and diphenylmercury are expected to be some of the major metabolites of phenylmercury acetate. As shown in Section B.4.1. phenylacetate is rapidly degraded to divalent or metallic mercury.

With regard to acute toxicity there is no big difference between methyl ($MeHg^+$) and phenylmercury ($PhHg^+$) but methylmercury is more persistent and has a greater potential to cause chronic toxicity (Walker, 2009). Alkylmercurials are more stable while aryl- and alkoxymercurials are easily transferred in vivo and in vitro to inorganic mercury. Alkylmercury compounds are more toxic than arylmercury compounds because arylmercury compounds have higher molecular masses that limit their permeation through biological membranes (Hempel *et al*., 1995).

To assess the toxicity of phenylmercury as a main metabolite of phenylmercury acetate, the following bioassays were performed by Hempel *et al*. (1995): Nematode Toxicity Assay (*Panagrellus redivirus*), Toxi-Chromotest, Resazurin Reduction Test, and the *Spirillum volutans* test. Hempel *et al*. (1995) used these bioassays to compare the toxicity of $PhHg^+$, $Hg2^+$ and $MeHg^+$. Various toxicological endpoints were used to evaluate the potential hazards arising from mercury-contaminated soils. The conducted tests are shortly described in the following:

Nematode Toxicity Assay (*Panagrellus redivivus*)

The nematode *Panagrellus redivirus* contains approximately 530 cells, organized in tissues and organs. The animal undergoes live-birth, with the newborn animals designated as second stage juveniles (J2s). Over a 96 h period, the newborn J2s grow through two additional juvenile stages (J3 and J4) to the adult stage. Each stage of the *Panagrellus redivivus* falls within a characteristic size and range. Under adverse conditions, the growth of the animals is arrested. Growth from J2 and J3 or from J3 of J4 requires very little gene activity. Animals that are alive but are remaining in the J2-J3 stage suggest chronic effects owing to low-grade toxicity. Growth from J4 to adult requires extensive gene activity. A specific inhibition of growth of J4s to adults can be used as an indication of potential genotoxicity on the test sample.

Toxi-Chromotest

This fairly rapid bacterial spectrophotometric assay in kit form is based on the ability of substances (toxicants) to inhibit the de nova synthesis of an inducible enzyme, beta-galactosidase, in a highly permeable mutant of E. coli. The sensitivity of the test is enhanced by exposing the bacteria to stressing conditions. The activity of the enzyme is detected by the hydrolysis of a chromogenic substrate. Toxic materials interfere with the recovery process and thus with the synthesis of the enzyme and the colour reaction.

Resazurin Reduction Test

Dehydrogenases are directly involved in many of the vital anabolic and catabolic processes of living organisms. Resazurin, an oxidation-reduction dye, reacts quantitatively with the

dehydrogenated form and thus can be used in the toxicity assessment of water-soluble chemical compounds or water samples. In this test a bacterium (Bacillus cereus) growth medium, resazurin and the sample are incubated together in a test-tube at room temperature for a period of 20-30 min. The reaction is stopped by extracting the dye with pentyl alcohol. The extract is measured spectrophotometrically at 610 nm for resazurin reduction caused by the microbial dehydrogenase activity. The extent of the inhibition of dehydrogenase activity, as indicated by the retardation of resazurin reduction, can be used to monitor toxic effects.

Spirillum volutans Test
Spirillum volutans is a large aquatic bacterium that is readily visible under low magnification. It has fascicle of flagella at each end, which, under normal conditions, form oriented revolving cones allowing the bacterium to move forward and reverse directions at will. During the reversing process the polar fascicles reorient simultaneously. To perform the test, *Spirillum volutans* is added to the sample and the mobility of the organisms is observed under a microscope. Toxicity is indicated by the non-coordination or death of the test organisms.

SOS-Chromotest
The use of *E. coli* for assessing the mutagenity/carcinogenity is based on the ability of the organisms to repair damage caused by chemicals. SOS-Chromotest measures the damage to desoxyribonucleic acid (DNA) through the action of an SOS-DNA repair system. In this assay, the SOS response of *E. coli* to DNA-damaging agents results in the biosynthesis of an enzyme (beta-galactosidase) the concentration of which can be determined spectrophotometrically after the addition of an o-nitrophenyl-β-galactopyranoside enzyme substrate (ONPG).

Table B-50 EC_{50}, LD_{50} and MEC_{90}* values of different mercury compounds for 4 bioassays (Hempel et al., 1995)

Mercury compound	Resazurin reductase test EC_{50} (mg l^{-1})	Spirillum volutans test MEC_{90} (mg l^{-1})	Toxi-Chromotest EC_{50} (mg l^{-1})	Nematode test LD_{50} (mg l^{-1})
Hg^{2+}	2.6	5	0.1	4
$PhHg^{+}$	1.05	0.5	0.04	3
$EtHg^{+}$	1	1	0.03	0.35
$MeHg^{+}$	0.75	0.1	0.02	0.015

*MEC90: An effective concentration of toxicant that inhibits 90% of reversing motility of *Spririllum volutans* after 120 min.

Table B-51 Toxicity factors of different organomercury compound, based on the toxicity of Hg2+ bioassays (Hempel *et al.*, 1995)

Toxicity factors	Resazurin reductase test EC_{50} (mg l^{-1})	Spirillum volutans test MEC_{90} (mg l^{-1})	Toxi-Chromotest EC_{50} (mg l^{-1})	Nematode test LD_{50} (mg l^{-1})
Hg^{2+}	1	1	1	1
$PhHg^{+}$	2.5	10	2.5	1.3
$EtHg^{+}$	2.6	5	3.3	11
$MeHg^{+}$	3.5	50	5	267

Table B-52 Genotoxic and toxic effects in the nematode test caused by organomercurials (Hempel *et al.*, 1995)

Species	Doses studied (mg L^{-1})	Doses of incomplete maturity* (EC_{50}/mg l^{-1})	Toxic doses EC_{50} (mg l^{-1})
$PhHg^{+}$	0.005-1.0	>1.0	3
$EtHg^{+}$	0.005-1.0	-	0.35
$MeHg^{+}$	0.005-1.0	>0.005	0.015

*Animals remaining in the J4 stage but no adults

The study reveals that methylmercury is the most toxic mercury species in these bioassays. In the Nematode test (LD_{50} mg l^{-1}) methylmercury is 276 times more toxic than inorganic mercury. Phenylmercury is more toxic than inorganic mercury. The toxicity factors range from 1.3 to 10 in the different bioassays based on the toxicity of inorganic mercury.
It is shown that the toxicity decreases as follows:
$MeHg^{+} > EtHg^{+} > PhHg^{+} > Hg^{2+}$ (Hempel *et al.*, 1995).

B.7.2.1.1 Toxicity to soil macroorganisms

The common form of mercury in soil is Hg (II). Methylmercury normally occurs in low percentages (0.5-1.5%), depending e.g. on soil moisture. Only few toxicity data are available for soil macroorganisms like earthworms and springtails concerning mercury toxicity although, some data are available for other terrestrial invertebrates. The sedentary and detrivorous earthworms seem to be more sensitive to metal polluted soils than the more mobile and migratory ground-living animals like ants, spiders, harvestmen and beetles (Bengtsson and Rundgren, 1984). Earthworms constitute over 90% of the invertebrate biomass in soils and are suggested to be an appropriate tool to predict bioaccumulation in the terrestrial food chain. Heavy metal accumulation in earthworm tissue was found to depend not only on the concentration of the substrate they consume, but also on ecological and species-specific physiological properties of different earthworms, such as efficiency of detoxification mechanisms, gut morphology, quantity of metal-binding ligands, consumption rates of the food material and feeding behavior. Effect concentrations are therefore species-specific and it is difficult to interpolate between different species (Ernst and Frey, 2007). Ernst and Frey (2007) showed that concentrations of Hg in earthworms were highest when the soil was Hg spiked compared to the applications with food (leaf or root litter) irrespective of the species investigated. Overall, the soil is the most important exposure medium of Hg for earthworms. In the study, it is also demonstrated that feeding behavior is one of the dominant factors determining heavy metal uptake in epigeic earthworms. The biota-soil accumulation factors (BSAF-related to the wet weight of organisms and dry weight of soil) for the transfer of Hg from soil to earthworms averaged 1.0 for Lumbricus terrestris and 2.3 for Octolaseon cyaneum. There exist species-specific physiological properties that may be important in regulating the accumulation of Hg in earthworm tissues and may have a stronger influence than the contrasting feeding behaviors.

Phenylmercury acetate
No data found

Phenylmercury propionate
No data found

Phenylmercury 2-ethylhexanoate
No data found

Phenylmercury octanoate
No data found

Phenylmercury neodecanoate
No data found

Degradation products of phenylmercury compounds
Diphenylmercury
No data found

Mercury (II) and methylmercury
Abbasi and Soni (1983) studied the influence of mercury chloride on the earthworm *Ocotchaetus pattoni*. The median lethal doses (LD_{50}) values were 2.39 ppm when the exposure period was 10 days and 0.79 ppm when the test lasts for 60 days. The mortality was less than 50% in the highest test concentration (5 ppm) at an exposure period of 5 days. At a mercury (II) concentration of 5 ppm within an exposure time of 10 days 100% mortality occurred. At the lowest concentration of 0.5 ppm 10% mortality was found within an exposure period of 10 days and 35% mortality after 60 days. No mortality occurred in the controls. In summary, increasing mortality occurred with increasing mercury concentrations and increasing duration of the test.

Lock and Janssen (2001) studied the effect of divalent mercury (II) on the earthworm *Eisenia fetida*, the enchytraeid worm *Enchytraeus albidus* and the springtail *Folsomia candida.* They found that the 21-day EC_{50} for the cocoon production of the earthworm *Eisenia fetida* was 9.16 mg Hg kg^{-1} dry weight. The 21-day NOEC was 10 mg Hg kg^{-1} dry weight and the 21-day LOEC was 18 mg Hg kg^{-1} dry weight.

Based on reproduction the 42-day EC_{50} for *Enchytraeus albidus* was 22.0 mg Hg kg^{-1} dry weight while its 21-day LC_{50} was 26.1 mg Hg kg^{-1} dry weight. No effects occurred at 18 mg Hg kg^{-1} dry weight (42-day NOEC). The 42-day LOEC was 32 mg Hg kg^{-1} dry weight (Lock and Janssen, 2001). The 28-day EC_{50} based on reproduction was 3.26 mg Hg kg^{-1} dry weight for the springtail *Folsomia candida.* The 28-day LOEL was 3.2 mg Hg kg^{-1} dry weight. In *F. candida* 100% mortality occurred when exposed to soil containing 10 mg Hg kg^{-1} dry weight. Less than 10% mortality occurred when the animals were exposed to soil containing 5.6 mg Hg kg^{-1} dry weight (Lock and Janssen, 2001).

Son *et al.* (2007) studied the effects of mercury (II) on the springtail *Paronychiurus kimi*. The 7-day LC_{50} was 3.9 mg kg^{-1} dry soil. The 28-day EC_{50} was 0.23 mg kg^{-1} dry soil based on reproduction. The study reveals that springtail populations decline at mercury concentration exceeding 2.0 mg kg^{-1} dry soil.

Holmstrup *et al.* (2008) found that mercury can influence the tolerance of low temperature stress in the the springtail *Folsomia candida*. The two stressors had synergistic effects. Furthermore, Slotsbo *et al.* (2009) studied the combined effects of mercury and heat. They

found synergistic effects between mercury and heat. Laboratory studies may underestimate the impact of a pollutant because no other stressors appear.

Earthworm immunobiology and immunotoxicology have been proposed for assessing risks to public and environmental health from hazardous waste sites and contaminated soil. The crucial parameters, including total coelomocyte count, coelomocyte viability, coelomocyte bacterial ingestion and killing, were reported to be inherently stable in unexposed control earthworms obtained and assayed at various seasons (Venables *et al.*, 1992) making these parameters suitable as endpoints for toxicity testing. Several variable factors play an important role in earthworm intoxication by heavy metals, including soil pH (Straalen and Bergema, 1995), metal solubility (Neuhauser *et al.*, 1984), metal bioaccumulation (Corp and Morgan, 1991), and metal retention by the surface mucus barrier covering the skin (Fleming and Richards, 1981). After *in vitro* exposure of coelomocytes of *Lumbricus terrestris* to mercury chloride and methylmercury chloride (10^{-4} M) the viability dropped, respectively, to 37.0% ± 7.0 and 18.0% ± 4.9 viable cells. The phagocyting index decreased significantly at 10^{-7} M for methylmercury and at 10^{-6} M for mercury chloride. The toxicity tests revealed that mercury causes a drastic inhibition of phagocytosis, accompanied by a relatively high cytotoxicity at higher concentrations of the metal. Earthworm species react differently when exposed to chemicals. For example, *Apporectadea caliginosa* was frequently the most sensitive species, *Lumbricus terrestris* intermediate and *Eisenia foetida* least sensitive. Some physiological response mechanisms to heavy metals were reported to be species-specific (Fugère *et al.*, 1996).

Tolerance of animals against metals is attributed to the duplication and higher transcription rate of metallothionein genes, metallothionein sequestering and metal-metallothionein adduct excretion, which was investigated on the cellular level (van Straalen and Roelofs, 2005). Synthesis of new enzymes is an energy demanding process indicating stress.

Some organisms show mercury resistance. In arthropods guts, mercury can be detoxified by mercury-resistant bacteria bearing the *mer* operon. The *mer* operon enzymatically reduces highly bioavailable Hg^{2+} into the volatile Hg^0 form, which evaporates from the bacterial cell (Barkay *et al.*, 2003).

Response to short-term Hg exposure in *Porcellio scaber* differs for animals from Hg polluted and unpolluted field locations. The animals and their gut microbiota from the Hg polluted location were less affected by Hg in a short-term feeding experiment than those from the unpolluted environment (Lapanje *et al.*, 2007).

Beyer *et al.* (1985) demonstrated that methylmercury can bioaccumulate in earthworms exposed to methylmercury-contaminated soil. Furthermore, they found a significant decrease in regeneration capacity at about 5.0 mg MeHg kg^{-1} dry weight. The bioaccumulative properties of Hg (II) are much lower than that of methylmercury. Ernst el al. (2008) found that BSAFs (biota to soil accumulation factors) for Hg were in the range of 1-15 depending on the earthworm species. Endogeic species had the highest BSAFs. For determining bioaccumulation factors, earthworm tissue concentrations should be primarily related to soil concentrations (Ernst and Frey, 2007). Burton *et al.* (2006) studied bioaccumulation of total mercury and methylmercury in the earthworm *Eisenia fetida* in contaminated soils. They found that BSAFs for total Hg ranged from 0.6 to 3.3. For methylmercury BSAFs ranged from 175 to 249. Total Hg concentrations ranged from 85 to 11542 µg kg^{-1} dry weight soil. Methylmercury concentrations ranged from 1.12 to 7.35 µg kg^{-1} dry weight soil.

B.7.2.1.2 Toxicity to terrestrial plants

Mercury may be directly taken up by plants and may subsequently lead to toxic reactions such as reduced root, shoot or leaf growth, internode development and other anatomical deficiencies (Han *et al*. 2006). Factors affecting plant uptake include external mercury concentration and exposure time, soil or sediment organic content, carbon exchange capacity, oxide and carbonate content, and redox potential (Crowder, 1991). Plants can take up mercury from soils into the roots and uptake from soils depends on the soil type. Uptake decreases with increasing content of organic matter (WHO, 1989). The absorption of mercury directly from the air through leaves via stomata is negligible for species such as beech and spruce (Schmidt, 1987) but important for pines and herbaceous plants (Mosbaek *et al*., 1988; Maserti and Ferrara, 1991). Bryophytes and lichenes take up metals only from water and air (Crowder, 1991). The bryophyte *Sphagnum sp.* bioconcentrates mercury up to 1200 µg g^{-1} (Siegel *et al*s, 1985). The wodden *Pinus sp*. also bioconcentrates mercury (Siegel *et al*., 1987).

Excessive concentrations of metals like mercury have many adverse effects on plants. Mercury can change the permeability of the cell membrane and it reacts with sulphydryl–groups. It can react with phosphate groups and active groups of ADP and ATP. Additionally, mercury can replace essential cations, which are needed for plant development.

Phenylmercury acetate
Phenylmercury acetate acts as an antitranspirant when applied to leaves. At concentrations of 10^{-5} – 10^{-3} M (3.4 - 337 mg/l) phenylmercury acetate the transpiration rate of lupines (*Lupinus termis* L.) decreased significantly (Ahmed *et al.*, 1987). PMA retards stomatal closing as well as stomatal opening. PMA may conceivably decrease the permeability of guard cell membranes to solutes, thereby retarding all stomatal movements that are osmotically induced (Davenport *et al.*, 1971). PMA treatment caused a decrease in chlorophyll content even at low PMA concentration (10^{-5} M, 3.4 mg/l). Considerable PMA toxicity was observed when the spraying solutions contained concentrations of 10^{-3} M (337 mg/l) and 10^{-4} M (33.4 mg/l), which resulted in a browning of leaves following PMA application (Waisel *et al.*, 1969).

Phenylmercury propionate
No data found

Phenylmercury 2-ethylhexanoate
No data found

Phenylmercury octanoate
No data found

Phenylmercury neodecanoate
No data found

Degradation products of phenylmercury compounds
Diphenylmercury
No data found

Mercury (II)

Cargnelutti *et al*. (2006) studied the effects of exogenous mercury chloride on changes in the enzymes catalase and ascorbate peroxidase, lipid peroxidation, chlorophyll content and protein peroxidation in cucumber seedlings (*Cucumis sativus L.*). Mercury chloride concentrations ranged from 0 to 500 µM in medium. The test lasted for 10 and 15 days, respectively. The growing seedlings absorbed mercury especially in their roots. Hg accumulation in the root system indicates that roots serve as a partial barrier to the transport of Hg to shoots (Cavallini *et al*., 1999). At all concentrations tested, a concentration-dependent reduction in root and shoot length could be noticed at both 10 and 15 days. At 50 µM $HgCl_2$ (, root growth (fresh weight) of 15-day-old seedlings increased, and at other concentrations, it was reduced. This might be due to a hormesis effect. Growth hormesis represents overcompensation due to a disruption in homeostasis. For 10-day-old seedlings, reduction in root and shoot fresh biomass was observed. After 15 days at all concentration except from 50 µM $HgCl_2$ (10 mg/l) a reduction in shoot fresh biomass was observed. Dry weight of roots increased at 500 µM (100 mg/l) both at 10 and 15 days, though at 250 µM $HgCl_2$ there was only an increase after 15 days exposure. Elevated lipid peroxidation occurred with increasing mercury concentration. Furthermore, protein oxidation levels increased. Chlorophyll content decreased between 250 and 500 µM $HgCl_2$. At 500 µM $HgCl_2$, catalase activity of 15-day-old seedlings was 51% lower than that of the control. At 250 µM $HgCl_2$, the seedlings showed the highest level of catalase activity. However, the catalase activity was also reduced at 50 µM $HgCl_2$.

Cho and Park (2000) studied the effects of mercury to tomato seedlings (*Lycopersicon esculentum* Mill.) where mercury was applied as mercury chloride in water. The tomato plants were watered with a 0, 10 and 50 µM mercury chloride solution. Hg increased with increase in external concentration and exposure time. Roots accumulated more mercury than the upper parts. After 20 days the mercury concentration in roots was about 27-fold higher than in shoots. The highest concentration in roots was 1418.9 µg g^{-1} dry weight, plants were treated with 50 µM (10 mg/l) Hg for 20 days. Depressions of shoot and root dry weight could be noticed. 50 µM Hg for ten days increased the level of endogenous H_2O_2. The H_2O_2 concentrations were much higher in roots than in leaves but effects of Hg on H_2O_2 level measured at day 10 was much higher in leaves than in roots. The activities of the antioxidant enzymes superoxide dismutase (SOD), catalase (CAT) and glutathione peroxidase (GPX) were increased by Hg-exposure estimated on fresh weight basis, depending on exposure time and treatment levels. Ten-day exposure to 10 µM (2 mg/l) Hg was enough to increase the activity of SOD, and the increased SOD activities paralleled the levels of formed H_2O_2 in leaves and roots.

Chen *et al.* (2009) examined bioaccumulation and physiological effects of mercury in the ferns *Pteris vittata* and *Nephrolepis exaltata*. The plants grew in a hydroponic solution containing $Hg(NO_3)_2$. The solutions contained free mercury concentrations of 0, 4.11 and 16.7 mg Hg l^{-1}. Both ferns accumulated high mercury concentrations in the roots (*P.vitatta*: 3534 mg kg^{-1} dry weight; *N. exaltata*: 2645 mg kg^{-1} dry weight) at the high concentration and 1298 and 1117 mg kg^{-1} dry weight, respectively at mercury concentrations of 4.11 mg Hg l^{-1}. Mercury was to a little extent transferred to the shoots. The shoots of *P. vittata* and *N. exaltata* contained 5.8 and 3.1 mg Hg kg^{-1} dry weight, respectively at the high concentration and 4.5 and 1.0 mg Hg kg^{-1} dry weight at the low concentration. Severe visual toxic symptoms such as withering, chlorosis and falling of leaves appeared in *P. vittata*, especially at 16.7 mg l^{-1} mercury level; in contrast, no toxic symptoms were observed for *N. exaltata*. Mercury exposure led to more pronounced phytotoxicity accompanied by stronger oxidative

stress in the shoots of *P. vittata* than in *N. exaltata*. *N. exaltata* established a more effective anti-oxidative system against mercury-induced oxidative stress than *P. vittata*. The content of H_2O_2 in shoots of *P. vittata* after three days was 87% and 126% compared to controls at 4.11 and 16.7 mg Hg l^{-1}. After seven days H_2O_2 content was 229% and 290% at 4.11 and 16.7 mg Hg l^{-1}. However, H_2O_2 concentration in *N. exaltata* did not show a significant change at either mercury level. Lipid peroxidation increased also significantly in *P. vittata* but not in *N. exaltata*.

Mathre and Chaphekar (1984) investigated the effects of mercury to the cereal *Pennisetum tyhoideum* Stapf. var PHB-14, the forage crop *Medicago sativa* L. var. Raska and the vegetable *Abelmoschus esculentus* Moench. var. Pusa-savni. Seeds were cultivated in sand and 150 ml of nutrient solution were added daily. The plants were transferred to clay jars containing nutrient solution mixed with $HgCl_2$ at the 4-leaf stage. The Hg-nutrient solutions contained 1, 10, 100 and 1000 µg l^{-1} Hg. The plants remained in the test concentrations for 24 hours. Afterwards, they were transferred to jars containing nutrient solution without Hg. After 24 hours, the visible leaf injury was recorded on a graph paper. The Leaf Injury Indices were calculated. Toxicity was based on nominal concentrations. At 1 µg l^{-1}, none of the plants showed foliar injury. From 10 µg l^{-1} upwards, intensity of injury increased with increased metal dose. The degree of sensitivity showed *P. typhoideum* to be most susceptible, followed by *M. sativa* and *A. esculentus*. Total chlorophyll content decreased with increasing metal concentrations and also the total dry matter of all three plants decreased. Subtle damage in terms of reduced chlorophyll content and reduction in standing phytomass of the plants was also observed even at 1 µg l^{-1}. Experiments showed that *Poa annua* can accumulate mercury when it was irrigated with mercury polluted water. Therefore, contaminated plants should not be used as fodder because they can carry mercury in the food chain. *P. annua* accumulates metals even in conditions of very low concentrations. In particular, mercury uptake takes place even with very low initial concentrations in water (Comino *et al.*, 2009).

Sheppard *et al*. (1993) investigated the sensitivity of *Brassica rapa* (Bird rape) and *Lactuca sativa* (lettuce) to mercury chloride in three different soil types. Experiments were performed with mercuric chloride ($HgCl_2$). As endpoints the height and biomass of the plants were used for *Brassica rapa*, as well as seed emergence and first blooming. For *Lactuca sativa* only seed emergence was recorded. Timing of bloom initiation and stem dry weight were the most sensitive endpoint for mercury effects in *Brassica rapa.* Of all tested soils the sandy soil showed toxic effects at the lowest mercury concentrations. No-effect concentrations (NOECs) in sandy soil were 22 mg/kg for stem dry weight (plant growth) and 10 mg/kg for first blooming of *Brassica rapa* and 460 mg/kg for seed emergence of *Lactuca sativa.* In garden and clay soils the NOECs were considerably higher.

B.7.2.1.3 Toxicity to soil microorganisms

Soil biology is an important component of soil quality and microorganisms play vital roles in soil fertility and primary production through organic matter decomposition and nutrient cycling. Chemicals can affect soil biota as well as the ecological processes regulated by these microorganisms. Soil may become contaminated with metals by a variety of anthropogenic sources. Various potentially toxic elements, including heavy metals, are present in industrial wastewater. Elevated concentrations of these compounds are known to affect soil microbial populations and their associated activities

Phenylmercury acetate

Ojo *et al*. (2007) found that the fungicide Ceresan (CAS number 8013-47-6) containing PMA completely inhibits the population of bacteria at 25 µg PMA g^{-1} soil, 50 µg PMA g^{-1} soil and 75 µg PMA g^{-1} up to 33 days after treatment (DAT). The lowest concentration (25 µg g-1 soil) is below the recommended application rate, the second (50 µg g^{-1} soil) equates the recommended rate of application and the third (75 µg g^{-1} soil) is above the recommended rate. The population of actinomycetes increased with days after treatment. Attention must be paid to non-target effects of pesticides. Especially, problems will occur if microbes are affected because they are essential for the soil's quality and vitality. Soil microorganisms act as decomposers and mineralizers. Microorganisms are necessary for the recycling of nutrients. Furthermore, several soil organisms such as nematodes and protozoa consume microorganisms. Rhizobia (diazotrophs) that are generally gram negative, motile and non-sporulating rods live symbioticaly with legumes and may also be affected by phenylmercury acetate. Many fodder plants like lupines and clover are legumes. Kanematsu *et al*. (1980) found that PMA causes DNA damage in Bacillus subtilis at 1 mM using the Differential Killing Assay.

Additionally, many plants live in association with specialized fungi. This association is called mycorrhiza. Ojo *et al*. (2007) found that the fungi population is completely inhibited at a concentration of 25 µg PMA g-1 soil. Recolonizing took place after 63 days after treatment. At higher rates of application (50 and 75 µg g^{-1} soil) recolonizing occurred also after 63 days after treatment but to a minor degree.

Ojo *et al*. (2007) tested also effects of PMA on protozoa. They showed that Ceresan completely inhibits protozoans throughout the period of 63 days and at all concentrations of application (25, 50 and 75 µg PMA g^{-1} soil). Protozoans are an important food source for microinvertebrates.

Ekundayo (2002) got similar results. He studied the effects of different pesticides on bacteria, actinomycetes, fungi and protozoa. It was found that Agrosan which contains PMA inhibited bacterial density from 4,600,000 to 220 cells g^{-1} soil. The fungicide was applied at the recommended rate of 50 µg PMA g^{-1} soil. Of the 11 pesticides investigated, PMA had the strongest adverse effect on bacteria. PMA eliminated protozoa totally and reduced fungal population from 34,000 to 60 cells g^{-1} soil. Actinomycetes were less susceptible to PMA. The population reduced from 340,000 to 4,800 cells g^{-1} soil. The results are in agreement with those of Ojo *et al*. (2007).

Odeyemi and Ogunledun (1983) found that a cowpea rhiozbium could not multiply in the presence of 0.3 µg ml^{-1} Agrosan. PMA affects the respiration by poisoning essential sulphydryl respiratory enzymes in bacterial and fungal cells (Cremlyn, 1978).

Summing up, PMA is toxic to soil organisms such as bacteria, protozoans and fungi. Harming soil microorganism by the use of PMA will have widespread impact on soil quality because organisms at the lower end of the food chain are affected. Therefore, all organisms of the soil food web will suffer. Different arthropods, nematodes and protozoans feed on bacteria. These organisms as bacteria themselves are important for degrading organic material.

Phenylmercury propionate

No data found

Phenylmercury 2-ethylhexanoate
No data found

Phenylmercury octanoate
No data found

Phenylmercury neodecanoate
No data found

Degradation products of phenylmercury compounds

Diphenylmercury
No data found

Mercury (II)
Abou-Shanab *et al*. (2007) studied the effect of nine metals (As, Cd, Cr, Zn, Hg, Pb, Co, Cu, Ni) to 46 soil bacterial cultures in agar medium. One culture collection strain, 30 strains from the rhizosphere of Alyssym murale and 15 strains from a Ni-rich soil were used. Hg was the most toxic element, 71% were sensitive to mercury. Mercury was inhibiting 7% of the bacterial isolated strains at 0.01 mM (2 mg l^{-1}). The bacteria were cultivated on tris-buffered low-phosphate agar (TBLPA) containing different metal concentrations. The NOEC was 0.005 mM (1 mg l^{-1}) Hg (II). The order of toxicity of the metals was found to be Hg > Cd > Co > Cr > Cu > As > Zn > Pb > Ni. In general, the toxic effect of these metals increased with increasing concentration. Some of the grampositive and gram-negative bacteria bearing the czc, chr, ncc and mer genes that are responsible for resistance to Zn, Cr, Ni and Hg, respectively, were highly resistant to Hg, Zn, Cr and Ni.

Oliveira and Pampulha (2006) examined key-microbiological parameters of a long-term polluted soil containing amongst others 109 mg mercury and 1558 mg arsenic per kg soil. They measured dehydrogenase activity, ATP content of the soil, number of culturable aerobic bacteria, actinomycetes, fungi, asymbiotic nitrogen-fixers. Large differences in all microbial properties between polluted and unpolluted sites were found. Asymbiotic nitrogen-fixers and heterotrophic bacteria were particularly sensitive to long-term pollution. As shown by Abou-Shanab *et al*. (2007) this study reveals that mercury was the most toxic element for a quantity of soil bacteria.

B.7.2.1.4 Toxicity to other terrestrial organisms

Phenylmercury acetate
The abilitiy of phenylmercury acetate to cause mutations has not been studied on soil organisms so far but some tests on *Drosophila melanogaster* were carried out. In *Drosophila melanogaster* fed with nutrient solution containing 20 g Ceresan (containing PMA) per liter, mutations occurred. To detect mutations the Sex-linked Recessive Lethals Assay was used (Gayathri and Krishnamurthy, 1985). Aneuploidy occurred in *D. melanogaster* testing with Non-disjunction Assay. The larvae were fed with a nutrient solution containing 0.32 mg PMA l^{-1} (Ramel and Magnusson, 1969).

Phenylmercury propionate
No data found

Phenylmercury 2-ethylhexanoate
No data found

Phenylmercury octanoate
No data found

Phenylmercury neodecanoate
No data found

Degradation products of phenylmercury compounds
Diphenylmercury
No data found

Mercury (II)
In the acridid grasshopper *Aiolopus thalassinus*, mercury prolonged the nymphal duration and the fresh body weight of the adults was significantly reduced in the F1 generation and the resulting F2 generation. The animals were fed on diets containing 0, 10, 30 and 70 mg kg^{-1} Hg (II). In the highest test concentration no F2 generation could develop because the grasshoppers of the F1 generation died within 4 weeks and did not lay eggs. The hatchability of the F1 generation was reduced but it was not different from the controls in the F2 generation (Schmidt *et al*., 1992).

Devkota and Schmidt (1999) found that at a concentration of 0.121 µg g^{-1} Hg (II) in the substrate, only 50.8% of the total eggs of *A. thalassinus* could undergo embryonic development (control: 62.17%), out of which 5.6% were found as dead nymphs trapped in the substrate and/or within the egg pods. At higher concentrations (0.605 to 12.1 µg g^{-1} Hg (II)) no eggs could develop to hatch. An accumulation factor for undeveloped eggs was calculated to range from 12.6 (in 12.1 µg g^{-1} Hg (II) substrate) to 42.5 (in 1.21 µg g^{-1} Hg (II) substrate) in egg pod treatment.

B.7.2.2 Calculation of Predicted No Effect Concentration (PNECsoil)

Due to lack of data and also due to the fate of phenylmercury compounds in the environment it is proposed to perform the quantitative risk assessment for environment on the basis of the inorganic mercury data. As the estimation of PEC-values is afflicted with great uncertainty, this dossier relies predominantly on the PBT-like property of the degradation/transformation product methylmercury. The calculation of PNEC-values as part of the quantitative risk assessment are presented in Appendix 1.

B.7.3 Atmospheric compartment

Biotic hazard
No information is available on biotic hazard of phenyl mercuric compounds on/to the atmosphere.

Abiotic hazard
No information is available on abiotic hazard of phenyl mercuric compounds on/to the atmosphere.

B.7.4 Microbiological activity in sewage treatment systems

B.7.4.1 Toxicity to aquatic micro-organisms

Phenylmercury acetate
Pauli and Franke (1971) studied the degradation of PMA using a sewage sludge inoculum at an initial concentration of 5 and 10 mg/L. It was shown that PMA degrades slowly resulting in the formation of inorganic mercury compounds at a rate of 50% and 60% removal after 7 days. The authors also conclude that the formation of diphenylmercury is not likely to have occurred due to the formation of the inorganic forms of mercury, although there is no details to describe which products are likely to have been formed. As this study is not based on any type of guideline study, the data cannot be used to derive a NOEC.

Table B-53 Toxicity to aquatic micro-organisms

Method	Results	Remarks	Reference
Degradation of PMA using a sewage sludge inoculum	An initial concentration of 5 and 10 mg/L was found to slowly degrade to inorganic mercury compounds at a rate of 50% and 60% removal after 7 days.		Pauli and Franke, 1971

Phenylmercury propionate, -octanoate, 2-ethylhexanoate and -neodecanoate
No data found.

Other mercury compounds
INERIS (2000) reports a (geometric) mean NOEC of 11 µg/L for inorganic mercury (based on 6 and 16 hr NOEC values). For organic mercury, INERIS (2000) provides a NOEC of 0.2 µg/l for bacteria (based on an 18 hr NOEC value).

According to the UNEP report (2002), mercury is toxic to micro-organisms and has long been used to inhibit the growth of bacteria in laboratory experiments (WHO/IPCS, 1990). This report also indicates that effects of inorganic mercury has been reported at concentrations of 5 µg/l in cultures of micro-organisms, and of organic mercury compounds at concentrations at least 10 times lower (WHO/IPCS, 1991).

B.7.4.2 PNEC for sewage treatment plant

As the estimation of PEC-values are afflicted with great uncertainty for phenylmercury compounds, this dossier relies predominantly on the PBT-like property of the degradation/transformation product methylmercury. No quantitative risk assessment for sewage treatment plant has been performed. Predicted no-effect concentrations (PNECs) for

sewage treatment plant have been generated on organic mercury and are presented in Appendix 1.

B.7.5 Non compartment specific effects relevant for the food chain (secondary poisoning)

B.7.5.1 Toxicity to birds

Phenylmercury acetate
Mullins *et al*. (1977) studied the effect of orally administered phenylmercury ammonium acetate on captive game farm pheasants (*Phasanius colchicus*). The fungicide was Mist-O-Matic was used (Hg equivalent 0.86%, Gustafson Manufacturing Company, Minneapolis, Minnesota). One group was fed with 20 mg Hg kg^{-1} body weight. PMA was administered in gelatine capsules. Controls got empty capsules. Each bird received the equivalent of the amount of fungicide required to treat approximately 1.4 liters of seed wheat for planting. Right after application the mercury levels rose sharply in kidney, liver and ovarian follicle samples. The mercury levels approached control levels after 2 weeks. Treated hens had decreases in egg hatchability, eggshell thickness, chick weight, and chick survival. No differences could be found in egg production, egg volume, fertility, or chick behavior. Hens that fed ad libitum on seed wheat treated with 14.18 grams per bushel showed no overt effects. The mercury levels of kidneys were increased.

To find the LD_{50} for phenylmercury acetate, hen pheasants were fed with encapsuled doses of 40, 60, 80, and 100 mg Hg kg^{-1} body weight. The LD_{50} was interpolated at 65 to 70 mg Hg kg^{-1} body weight. Miller *et al*. (1960) found similar results for domestic chicken. They found a LD_{50} of 60 mg Hg kg^{-1} body weight.

Grolleau and Giban (1966) studied the effects of different pesticides on different bird species. For the Partridge (*Perdix perdix*) the lethal doses of PMA ($LD_0 - LD_{100}$) for a single ingestion ranged from 35-45 mg Hg kg^{-1} body weight. The Bantam (Gallus gallus) was much less sensitive. The $LD_0 - LD_{100}$ ranged from 200-290 mg Hg kg^{-1} body weight. When the phenylmercury acetate was apportioned into three doses the lethal dose was in the range of 40-80 mg Hg kg^{-1} body weight for the Partridge and in a range of 170-220 mg Hg kg^{-1} for the Bantam. The results reveal that the toxicity of phenylmercury acetate differs highly between the two bird species. When the three doses were applied the lethal dose for the Partridge increased while it decreased in the Bantam. The LD values should be treated as approximate values because they were shown graphically.

Single dose studies are not very useful for assessing the risk of a chemical for the terrestrial environment. However, these studies show that phenylmercury is toxic to birds. PMA affects reproduction and survival. It is also shown that single toxicity values should be treated with care because of high inter-specific differences.

Phenylmercury propionate
No data found

Phenylmercury 2-ethylhexanoate
No data found

Phenylmercury octanoate
No data found

Phenylmercury neodecanoate
No data found

Methylmercury
Many seabirds often contain high mercury concentrations. They feed on fish and other marine organisms. Fish is the most relevant source of mercury for seabirds. It often contains high amounts of the highly lipophilic and persistent methylmercury. Therefore, bioaccumulation and biomagnification of mercury occurs. Birds that live close to contaminated lakes and feed on mercury-contaminated freshwater fish contain also high amounts of mercury.

Captive American kestrels (*Falco sparverius*) were fed on diets containing 0, 3, 6 or 12 ppm methylmercury dry weight (nominal concentrations). Kestrels are usually predators of small mammals, lizards or large insects but are often used as experimental animals. All the raptors showed signs of neurotoxicity at the 12 ppm diet after 26 days. All animals died in 39 to 49 days. One male bird died after 75 days fed with 6 ppm diet. Signs of neurotoxicity occurred in several kestrels after 45 days. None of the birds fed with 3 ppm diet showed signs of neurotoxicity or died. After 59 days of exposure the mercury concentrations increased with increasing dietary concentrations. Mercury concentrations in liver, kidney, and blood were analyzed. Tissue concentration of mercury increased over time in birds fed diets with 6 ppm mercury. Kestrels were dissected at day 8, 15, 29 and 59. At day 59 the mercury concentrations in liver, kidney and whole blood were 57, 46 and 45 ppm, respectively. Two pairs laid eggs. The first pair was fed with 3 ppm diet and the second one with a 6 ppm diet. Mercury concentrations in eggs were 8.3 and 18.1 ppm wet weight. The feather concentrations of feathers grown during mercury exposure were 275 ppm for birds fed with 3 ppm diet and 542 ppm for kestrels fed with 6 ppm diet (www.epa.gov, 2009).

The breeding success of 60 kestrel pairs was studied. They were fed on diet containing sublethal concentrations of methylmercury chloride. Eggproduction, incubation performance and the number and percentage of eggs hatched decreased markedly between 3.3 and 4.6 mg kg^{-1} dry weight. Nestlings fledged were reduced at 0.7 mg kg^{-1} dry weight. Further decline occurred between 2 and 3 mg kg^{-1} dry weight. Total fledging failure occurred at ≥4.6 mg kg^{-1} dry weight. Population decline would be of concern with birds feeding on diet containing 0.7 mg kg^{-1} dry weight. Accumulation was especially high for kestrels. Lower accumulation factors were reported either for wild birds and captive nonraptors fed on commercial food containing 5 mg kg^{-1} (www.epa.gov, 2009).

Heinz (1979) studied the effect of a 0.5 ppm methylmercury diet to three generations of mallard ducks (Anas platyrhynchos). The percentage of eggs outside the nestboxes was higher than in controls. Fewer ducklings hatched in the mercury treated group. A small amount of eggshell thinning was noticed. Ducklings were less responsive to tape-recorded maternal calls but they were hyper-responsive to a frightening stimulus in avoidance tests.

Field observations are mentioned in literature that indicate that in certain fish-eating avian species (divers, sea eagle, fish eagle), intoxications and reproductive impairment were noted after eating fish that contained methylmercury at concentrations of 0.2 to 0.7 mg/kg, Euro Chlor (1999).

Total mercury

Nicholson and Osborn (1984) examined ten juvenile starlings (*Sturnus vulgaris*) approximately 3 month old when they were netted. For eight weeks they were fed a libitum on a mercury containing diet. At the end the birds were killed and their kidneys were examined. It was found that 1.1 mg kg^{-1} food was sufficient to damage different cell types in the kidney. The starlings fed on a commercial animal feed. The birds showed no signs of toxicity during the experiment and no abnormal morphological features were noticed on dissection. In this study it was not tested in which form mercury occurred in the diet.

In birds, adverse effects of mercury on reproduction can occur at egg concentrations as low as 0.05 to 2.0 mg/kg (wet weight). Eggs of certain Canadian species are already in this range, and concentrations in the eggs of several other Canadian species continue to increase and are approaching these levels (UNEP, 2002).

The chance of mercury contamination for birds that feed on terrestrial insects and plant material is lower than for fish-eating birds. In terrestrial environments methylmercury is synthesized to a lesser degree than in aquatic environments. Some terrestrial birds like the tree swallows (*Tachycineta bicolor*) feed on emergent aquatic insects. Brasso and Cristol (2008) studied the effect of mercury exposure on reproductive success of tree swallows. The experimental swallow population was located in the headwaters of the Shenandoah River, Virginia, USA. One tributary, the South River, was contaminated with mercury before 1950. The female swallows nesting within 50 m of this river had a significantly elevated blood and feather total mercury. The mean blood concentration was 3.56 ± 2.41 ppm wet weight. The swallows of the reference sites had a mean blood concentration of 0.17 ± 0.15 ppm. The feather concentration was 13.55 ± 6.94 ppm while the birds on the reference sites had a mean feather concentration of 2.34 ± 0.87 ppm. Insects collected by the swallows averaged 0.97 ± 1.11 ppm dry weight total mercury. The mercury concentrations of insects on the contaminated area were significantly higher than on reference sites. The female swallows had fewer fledglings in 2006 in the contaminated area but the effect occurred only in young females. The young bird may already have been stressed by inexperience.

Elevated mercury levels can also occur in birds with no relation to aquatic environments as the Bicknell's trush living in a montane environment. Methylmercury can be present in forest leaves and leaf detritus; saturated soils and other moist microhabitats may also contribute to methylmercury availability (Rimmer *et al*., 2005). Mercury levels in non-aquatic birds have been poorly studied and very little is known about effects of mercury in songbirds.

B.7.5.2 Toxicity to mammals

Terrestrial mammals can be exposed to mercury by ingestion of mercury-contaminated food or drinking water. Inhalation may also be an exposure pathway.

Little is known about the bioaccumulation of mercury and methylmercury in terrestrial invertebrates. Limited studies of food chain transfer of mercury from contaminated surface soil to small mammals that consume earthworms as a part of their diet indicate that inorganic mercury concentrations in biota do not exceed concentrations in the soil (Bull *et al*., 1977, Talmage and Walton, 1993). Talmage and Walton (1993) found bioaccumulation of mercury over lower trophic levels when they examined kidneys of the shrew *Blarina brevicauda*.

Earthworms are the main part of their diet. They did not accumulate mercury themselves but contain high amounts of contaminated soil. The mean kidney concentration of *Blarina brevicauda* was 38.8 µg g^{-1} and the mean diet concentration was 8.82 µg g^{-1}. Thus, the mean transfer coefficient is 4.40.

Phenylmercury acetate
Hartke *et al*. (1976) studied the effects of intraperitoneal applied phenylmercury acetate in common prairie voles (*Microtus ochrogaster*). This application form is not natural but phenylmercury acetate which is taken up via food is readily and unaltered resorbed from the gastrointestinal tract (Aaronson and Spiro, 1973). Therefore, this study can be taken into account. In this study, embryotoxicity was of main interest. Single doses of PMA were applied at day 8, 9 or 10 of gestation period. Additionally, a dose-stage relationship for 0.5 mg kg^{-1} body weight applied at days 7, 11 or 12 was studied. It was found that at doses of 0.125, 0.25, and 0.5 mg PMA kg^{-1} body weight applied at day 8 lead to normal embryos but resorption sites were found. If an embryo dies it can be resorbed by the surrounding tissue. Afterwards, visible resorption sites can be found in the uterus. In uteri of females treated with 1, 2, and 5 mg PMA kg^{-1} body weight no living fetuses were found but all had resorption sites. Animals treated with 0.06, 0.125, 0.25, and 0.5 mg PMA kg^{-1} at day 9 of gestation period had normal fetuses. Resorption sites were found in the same uterus. Females treated with 1, 2, and 5 mg PMA had no living fetuses but all had resorption sites. When the same doses were applied at day 10 of gestation period the there were no resorption sites at concentrations of 0.06, 0.25, and 1.25 mg PMA kg^{-1} body weight. When doses of 1, 2, or 5 mg were applied no fetus was alive and resorption sites could be detected. The dose-stage relationship study resulted in normal fetuses but also resorption sites when given on day 7 and 11. Normal fetuses and no resorption sites could be found on day 12.
This study shows that PMA has embryocidical effects. Mature fetuses are better protected than young fetuses. Following this study, the LOAL for a single dose is 0.06 mg PMA kg^{-1} body weight (i.p.).

Fitzhugh *et al*. (1950) studied chronic oral toxicity of phenylmercury acetate in rats. This study is described in detail in Section B 5.6. Rats were fed on a phenylmercury acetate containing diet for two years (0, 0.1, 0.5, 2.5, 10, 40, or 160 mg of mercury in the form of phenylmercury aceate per kg diet). The amount of as little as 0.5 ppm mercury as phenylmercury acetate resulted in kidney damage in females after 2 years. At 0.1 ppm no differences could be detected between the controls and the treated animals. Higher doses above 2.5 ppm mercury resulted in renal lesions in males and females. EPA assumes a NOEL of 0.1 ppm (www.epa.gov, 2010). They assume that rats consume about 5% of their body weight in food per day. This results in a NOEL of 0.0084 mg PMA kg^{-1} body weight for a chronic diet. Due to the fact that higher mercury levels were found in kidneys and livers of rats fed on a 0.1 ppm diet it is suggested that the long-term study in the rat failed to demonstrate a NOEL (www.inchem.org).

Phenylmercury propionate
No data found

Phenylmercury 2-ethylhexanoate
No data found

Phenylmercury octanoate
No data found

Phenylmercury neodecanoate
No data found

Mercury (II)
Laboratory studies showed that mercury chloride causes oxidative stress in male rats. Boujbiha *et al*. (2009) fed male rats on diets containing 0, 50 and 90 ppm $HgCl_2$ for 90 days. Mercury was orally administrated through drinking water. The absolute and relative wet weight of the testes increased and the absolute and relative wet weight of the accessory sex glands. Mercury chloride caused perturbations in antioxidant defense and a significant dose-dependent increase in the testicular lipid peroxidation as a consequence of pro-oxidant exposure. Free radical formation increased relative to loss of antioxidant defense system. Testes were susceptible for oxidative damage leading to their functional inactivation.

The effects of chronic exposure to mercury chloride were studied by Heath *et al*. (2009). They exposed female Sprague-Dawley rats to 1 or 2 mg mercury chloride per kg body weight and day. At 90 days they were mated with untreated male rats. The females were dissected at day 13 of the gestation period. Number of implantations and non-viable implantations in the uterus were determined. There were no physical signs of Hg intoxication except for weight gain. Females in the high mercury chloride group had significantly fewer implantations, with significantly more non-viable implantations in the low and high mercury chloride groups compared to controls. Hormone levels were influenced in the high mercury chloride group. Females had lower levels of progesterone and higher levels of pituitary luteinizing hormone (LH). The study showed that also low levels of mercury chloride chronically applied produce disruption of implantation and fetal viability. Changes in hormone levels indicate that mercury chloride may have a disruptive effect in corpora lutea which manifests itself after ovulation.

Methylmercury and Mercury (II)
Methylmercury biomaginification is of lesser concern in strictly terrestrial environments. A special case exists when terrestrial carnivores consume prey that has accumulated mercury originating from aquatic sources. Biomagnification of mercury can occur when these animals are prey of e.g. raptors. Minks are generalists but feed often on fish. Aulerich *et al*. (1974) studied the effects of a methylmercury and a mercury chloride diet. A 5 ppm methylmercury diet was lethal to all animals in about a month. Animals lost weight and were anorectic. They showed signs of incoordination, had tremors and paroxysmal convulsions. The latency period lasted for 24 days. The animals had elevated concentrations of mercury in liver, kidney, muscle, spleen, brain, lung, and heart tissue. A 10 ppm mercury chloride diet had no obvious effects. But the mercury levels in kidney were elevated. Only one mink fed on mercury chloride diet was analyzed. Therefore, no mean concentrations are available. In this case long-term studies would be necessary to study the effects of mercury chloride. This study allows no predictions of the chronic effects of mercury chloride. Furthermore, the effect of only one concentration of methylmercury and mercury chloride was studied. Therefore, no dose-response relationship is available. Minks and otters are semi-aquatic top predators. They are at risk for chronic mercury exposure. In the long-term sub-lethal effects can lead to changes in population dynamics (Kruuk *et al*., 1997; Evans *et al*., 1998). High levels of Hg in mink and otters have been suggested as being responsible for declines in population, and in some cases disappearances in many parts of their range (Osowski *et al*., 1995; Kruuk *et al*., 1997).
Klevanic *et al*. (2008) found that mercury concentrations were related to the presence of the parasite Dioctophyma renale in mink.

Histopathological analyses of different animals with elevated mercury levels revealed neurodegenerative changes in the cerebral cortex (Wolfe *et al*., 1998). Brain concentrations of 1 mg g^{-1} wet weight in Nova Scotia captive mink caused changes in brain neurochemistry (Basu *et al*., 2006).

B.7.5.3 Calculation of PNEC oral (secondary poisoning)

The phenylmercury compounds are degraded to hazardous degradation products, i.e. inorganic mercury compounds and elemental mercury, which can be transformed to methylmercury. This dossier relies predominantly on the PBT like property of the degradation/transformation product methylmercury. PNEC's for PMA and degradation/transformation products have also been derived and is presented in Appendix 1. Because of lack of data a PECoral has not been calculated (neither for the phenylmercury compounds themselves or the degradation/transformation products). A quantitative risk characterization for secondary poisoning could not been performed.

B.8 PBT and vPvB assessment

B.8.1 Assessment of PBT/vPvB properties – Comparison with criteria of Annex XIII

The phenylmercury compounds have been assessed according to the criteria for PBT or vPvB substances in REACH Annex XIII and the Guidance document on PBT assessment.

Possible transformation or degradation products[8] that may have PBT/vPvB properties must also be considered. According to the Guidance document on PBT Assessment, chapter R.11.1; "If the substance contains one or more constituents with PBT/vPvB properties in individual amounts ≥ 0.1 % (w/w) or if transformation/degradation products with the respective properties in individual amounts ≥ 0.1 % are being generated, the substance must be treated like a PBT/vPvB with regard to emission estimation and exposure control.

B.8.1.1 Persistence

According to REACH Annex XIII and the guidance document on information requirements and chemical safety assessment Section C: PBT Assessment; A substance is assessed to be persistent when the half-life in fresh- or estuarine water is higher than 40 days or in soil and fresh- or estuarine water sediment is higher than 120 days. For marine water a half-life higher than 60 days or in marine sedimenta half-life higher than 180 days fulfils the persistence criterion.

Phenylmercury compounds

Experimental data on the persistence of the selected phenylmercury compounds was only found for phenylmercury acetate (see Section B.4 for comprehensive degradation data and references).

Phenylmercury acetate as a salt-like compound is expected to dissociate to the phenylmercury cation and the corresponding carboxylate. Dissociation of phenylmercury acetate is the initial reaction for the chemical and biological degradation of phenylmercury acetate.

For abiotic degradation, half lives in water are between 16 and 39 hours. In soils, chemical degradation is of minor relevance and occurs only in basic soils.

Available literature on the biodegradation of phenylmercury acetate indicates that microorganisms are capable to cleave the phenyl-mercurial bond of the phenylmercury cation. It is reported that phenylmercury acetate is rapidly degraded in waters by mercury tolerant microorganisms to metallic mercury, divalent mercury and volatile diphenylmercury. Half lives for degradation of the phenylmercury cation in waters are within hours to days, however, the available data is based on experiments with bacterial cultures. In sediments, at aerobic conditions, phenylmercury acetate is easily biodegraded within days and weeks. Anaerobic degradation of phenylmercury is expected to occur more slowly. Degradation rates of phenylmercury acetate in soils differ between soils, and half lives ranging from some days to

[8] According to REACH Annex XIII and the Guidance on PBT assessment, the PBT and vPvB criteria do not apply to inorganic substances but applies to organo-metals.

several weeks are reported. Degradation is closely related to physical-chemical conditions in soil and high sorption capacity of soil retard degradation.

The results cited above for phenylmercury acetate indicate that half-lives in waters, sediments and soils are below the persistence criterion.

Dissociation of phenylmercury proprionate is very similar to that of phenylmercury acetate. For the other organomercuric compounds (2-ethylhexanoato)phenylmercury, phenylmercury octanoate and phenylmercury neodecanoate no data on these compounds were found. According to theoretical calculations all five phenylmercury compounds (phenylmercury acetate, propionate, 2-ethylhexanoate, octanoate and neodecanoate) are salt-like substances that dissociate to phenylmercury and the corresponding carboxylate (see B.4). More than 90% of the compound is dissociated in environments with a pH value between 5 and 9. At these pH values phenylmercury is mainly present as phenylmercury hydroxide. The calculated average atmospheric lifetime of gaseous phenylmercury carboxylates is around 1 day.

The initial degradation reactions in the environment appear to be dissociation into phenylmercury and a carboxylate and/or cleavage of the phenyl-mercury bond in the presence of light. Therefore it is considered likely that the propionate, phenylmercury octanoate, (2-ethylhexanoato) phenylmercury and neodecanoate salts of phenylmercury will not behave very differently from the acetate with regard to transformation in the environment. The resulting phenylmercury cation is common for all five compounds.

Based on the above information, phenylmercury acetate, phenylmercury propionate, (2-ethylhexanoato)phenylmercury, phenylmercury octanoate and phenylmercury neodecanoate is not considered to fulfill the persistence criterion in REACH.

Degradation/transformation products

One of the main degradation/transformation products of the phenylmercury compounds in the aquatic environments is methylmercury, which has to be assessed against the PBT-criteria. The occurrence of methylmercury in aquatic system is the result of methylation of mercury and demethylation of methylmercury. Formation and degradation of methylmercury occur simultaneously. Methylation of mercury occur biologically by microorganisms primarily in sediments and is favored by anaerobic conditions (Pak and Bartha, 1998; Korthals and Winfrey, 1987; Stein *et al*., 1996). Methylation activity is usually much less in the water column (Pak and Bartha, 1998; Korthals and Winfrey, 1987; Stein *et al*., 1996). Methylmercury formed in the aquatic environment is biologically demethylated by microorganisms. Demethylation occurs in both aerobic and anaerobic conditions, although greater demethylation has been observed under aerobic conditions (Pak and Bartha, 1998; Korthals and Winfrey, 1987; Stein *et al*., 1996). According to Stein *et al*. (1996), biological demethylation occurs at a much lower rate than methylation. The net amount of biologically available methylmercury is a function of the rate of methylation and the rate of demethylation.

Because of the contrary processes of methylation and demethylation, the persistence of methylmercury in the environment cannot be assessed by degradation rates of methylmercury but on the ratio between methylation rate and demethylation rate. Methylation exceeds demethylation in surface layers of organic sediments with a high microbial activity. Here and in adjacent water layers methylmercury is continuously available for uptake in aquatic organisms. Most of the methylmercury that is found in fish tissues is covalently bound to

protein sulfhydryl groups. This binding results in a long half-life for elimination (about two years). Because of its high biological half-life it persists in organisms and biomagnifies in foodchains (Stein *et al*., 1996). Estimates for the biological half-life of methylmercury in humans range from 44 to 80 days (UNEP, 2008).

A direct comparison of degradation half-lives in water and sediment with the P criteria in Annex XIII is not relevant since both methylation and demythylation occur in water and sediment. The environmental conditions in surface near, organic sediments and adjacent water layers imply that demethylation occurs at a much lower rate than methylation. Moreover, methylmercury is available for uptake in aquatic organisms and because of its high biological half-life it persists in organisms and biomagnifies in foodchains. From the data available and due to the methylation – demethylation pattern the persistence criterion cannot be confirmed. However, the fact that demethylation occurs at a much lower rate than methylation in organic sediments (primarily) under anaerobic conditions and the fact that methylmercury has a high biological half-life should be judged as of equivalent concern. The cycling of mercury means that the source of methylmercury in the environment is always present once released. The measured environmental concentrations of mercury and methylmercury and the increasing trends of methylmercury levels in biota are of concern.

B.8.1.2 Bioaccumulation

According to REACH Annex XIII and the guidance document on information requirements and chemical safety assessment part C: PBT Assessment; A substance is considered to be bioaccumulative if the experimental bioconcentration factor is determined to be >2000. A substance is considered to be very bioaccumulative (vB) if the experimentally determined BCF >5000.

Phenylmercury compounds

Based on experimental data a bioaccumulation factor of 80, 90 and 100 (for aquatic concentrations of 5, 10 and 20 µg/l, respectively) was found for phenylmercury acetate. Bioconcentration factors were also estimated with QSAR. For phenylmercury acetate a BCF of 100 was estimated.

No experimental data are available for the other compounds. Estimated BCFs for the five phenylmercury compounds in water with pH5 are between 100 and 1579 and the criterion for bioaccumulation (B) is not fulfilled by phenylmercury compounds themselves.

The estimated BCF-values in water with pH5 were 100, 445,487,1579 for the phenylmercury propionate, (2-ethylhexanoato)phenylmercury, phenylmercury octanoate and phenylmercury neodecanoate respectively (see Section B.4 and Appendix 2).

Based on the available information phenylmercury acetate, phenylmercury propionate, (2-ethylhexanoato) phenylmercury, phenylmercuric octanoate and phenylmercury neodecanoate are not considered to fulfil the bioaccumulation criterion in REACH Annex XIII.

Degradation/transformation products

The inorganic mercury species eventually formed by biotransformation reactions (as described in Section B.4) can, under anaerobic conditions, undergo bacterially mediated

methylation to methylmercury and it is likely that the eventual transformation of the phenylmercury compounds to methylmercury will be greater than 0.1% (locally dependent on the microbial systems available for transformation). Thereby, the release of all the above substances also implies a risk of formation of methylmercury, which is known to biomagnify strongly in aquatic food webs via the diet. Bioconcentration factors as high as 107 has been measured (Weiner *et al*., 2003). Hill *et al*. (1996) showed that the bioconcentration factors for methylmercury increased between 0.5-1.5 log units per lower trophic level in a freshwater ecosystem. The high bioaccumulation potential of methylmercury is substantiated by BCFs for methylmercury in fish of 8 140 (geometric mean for fish) up to 85 700 for rainbow trout (Oncorhynchus mykiss), reported in the substance data sheet for mercury for the Water Framework Directive (WFD). The Scientific Committee on Health and Environmental Risks (SCHER) (2008) refers in its opinion on the environmental risks and indirect health effects of mercury in dental amalgam (2008) to reported bioaccumulation factors (BAF) measured in the field for fish species collected at different locations that range from about 20 000 to over 20 000 000. This shows that methylmercury is biomagnified significantly through the food web. In the literature field observations are mentioned that indicate that in certain fish-eating avian species (divers, sea eagle, fish eagle), intoxications and reproductive impairment were noted after eating fish that contained methylmercury at concentrations of 0.2 to 0.7 mg/kg (Eurochlor 1999).

These data clearly shows that methylmercury should be considered as bioaccumulative (B) and very bioaccumulative (vB).
According to the revised annex XIII of REACH other information on the bioaccumulation potential such as measured elevated levels in biota, compared to levels in their surrounding environment, can be provided. Detection of elevated mercury levels in fish show that in Scandinavia and North America elevated concentrations of Hg is often found in Northern pike and perch, and the concentrations are often above the limit recommended for human consumption concentrations. Mercury concentrations in surface waters in remote areas are usually lower than the WFD environmental quality standard (EQS[9]) (0.05 μg/l). However, many of these waters have fish with Hg concentrations substantially higher than recommended limits for human consumption (a maximum level of 0.5 mg/kg mercury applies to fishery products) and the WFD EQS for Hg in fish (0.02 mg/kg), which is exceeded for most fish all over Scandinavia.

This is confirmed by monitoring data from Sweden and Norway. During the last decade there has been an increasing trend in the mercury levels in inland fish in the majority of lakes in Sweden. Although the atmospheric depositions have declined, the depositions are still high. The levels in fish are currently about 3-5 times higher than the estimated background levels. In another study of trout from 17 different Norwegian lakes the concentration of mercury was determined in 223 trout, of which the populations in 14 of these had been investigated for mercury in the period 1988–2001. On average, the concentration had increased by approximately 23%, from 0.118 mg/kg to 0.145 mg/kg, which exceeds the WFD EQS for Hg in fish (0.02 mg/kg) for all analyzed fish.

Also data from the past few decades show that mercury levels are increasing in some Arctic biota, in particular in marine birds and mammals from areas in Canada and West Greenland (AMAP 2007).

[9] EQS: Environmental Quality Standard

B.8.1.3 Toxicity

According to REACH Annex XIII and the guidance document on information requirements and chemical safety assessment Part C: PBT Assessment; A substance is considered to be toxic (T) if the long term aquatic NOEC for marine or freshwater organisms is <0.01 mg/l, or if the substance is classified as carcinogenic (Cat 1 or 2), mutagenic (Cat. 1 or 2) or as toxic for reproduction (Cat 1, 2 or 3). Or in addition, if there is other evidence of chronic toxicity (i.e. identified by the classifications: T, R48 or Xn, R48 according to Directive 67/548EEC) or as STOT RE 1, H372 or as STOT RE 2, H373 according to CLP Regulation (EC) No 1272/2008 (cf. CLP Regulation article 58).

Phenylmercury compounds

According to the data presented in Section B.7, the most sensitive and robust data set which was chosen for the derivation of the PNEC was a *Daphnia magna* reproduction test which indicated a NOEC of 1.12 µg/L on survival. This is lower than the cut off value for assigning if a substance should be classified as Toxic (<0.01 mg/L)) and therefore PMA should be assigned as a toxic substance. No toxicity data are available for the other four compounds.

PMA is classified and labelled in EU as T;R25-48/24/25 C;R34 N;R50/53 according to Annex I to directive 67/548/EC and as Acute Tox. 3, H301; STOT RE 1, H372; Skin Corr. 1B, H314; Aquatic Acute 1, H400; Aquatic Chronic, 1H410 according to Annex VI to CLP.

The other phenylmercury compounds are classified according to the group entry (organic compounds of mercury with the exception of those specified elsewhere in this Annex) as: T+; R26/27/28 R33 N; R50-53 according to Annex I to directive 67/548/EC and as Acute Tox. 2, H330; Acute Tox. 1, H310; Acute Tox. 2 , H300; STOT RE 2 , H373; Aquatic Acute 1, H400; Aquatic Chronic 1, H410 according to Annex VI to CLP.

According to the EU classification of PMA (T, R48 and STOT RE 1, H372) and of the other phenylmercury compounds (STOT RE 2), phenylmercury acetate, phenylmercury propionate, (2-ethylhexanoato) phenylmercury, phenylmercury octanoate and phenylmercury neodecanoate fulfil the T criterion in REACH Annex XIII.

Degradation/transformation products

According to REACH Annex XIII (revised) and the Guidance documents the PBT/vPvB assessment shall also take account of the PBT/vPvB properties of any transformation/and or degradation products. One of the main degradation/transformation products of the phenylmercury compounds in the aquatic environment is methylmercury, which has to be assessed against PBT criteria.

According to data presented in Section B.7, the most robust data set for methylmercury indicated that the NOEC was 0.26 µg Hg/l based on survival from a *Daphnia magna* reproduction test. This indicates that methylmercury should be classified as a toxic substance (T) as this NOEC for long term toxicity is significantly below the cut off value for T classification (i.e. <10 µg/l) according to Annex XIII.

According to the revised annex XIII of REACH results from long term or reproductive toxicity testing with birds can be considerd for the assessment of the toxicity property. Methylmercury is highly toxic to birds described in literature where field observations indicate that in certain fish-eating avian species (divers, sea eagle, fish eagle), intoxications

and reproductive impairment were noted after eating fish that contained methylmercury at concentrations of 0.2 to 0.7 mg/kg. This is affirmed by effects of 0.5 mg/kg methylmercury diet on reproduction and behaviour of three generations of mallard ducks *Anas platyrhynchos* and reproductive toxicity of 0.7 mg/kg methylmercury to the falcon *Falco sparvinus*.

The classification of methylmercury is agreed up on by TC C&L. The concluded classification from TC C&L according to directive 67/548/EC is:

Carc. Cat 3; R40: Limited evidence of a carcinogenic effect
Muta. Cat 3; R68: Possible risk of irreversible effects
Repr. Cat 1; R61: May cause harm to the unborn child
Repr. Cat 3; R62: Possible risk of impaired fertility
T+; R26/27/28: Very toxic by inhalation, in contact with skin and if swallowed
T; R48/25: Toxic: danger of serious damage to health by prolonged exposure if swallowed
R64: May cause harm to breast-fed babies

Based upon the provisionally agreed classification of methylmercury as Repr. Cat 1; R61, Repr. Cat 3; R62 and T; R48/25 methylmercury fulfils the criteria for toxicity according to Annex XIII.

B.8.1.4 Conclusion PBT assessment

Phenylmercury compounds

A summary with available test data and calculated data for the five phenylmercury compounds in relation to PBT criteria has been compiled.

Annex-XIII criteria	**Phenylmercury acetate**	**Phenylmercury propionate**	**Phenylmercury 2- ethylhexanoate**	**Phenylmercury octanoate**	**Phenylmercury neodecanoate**
P Half-life, fresh water > 40 d Half-life, fresh water sediment > 120 d	Half-life within hours to days in water Half-life < 120 d in fresh water sediment	Rapid dissociation into phenylmercury cation and carboxylate anion. Rapid hydrolysis to phenylmercury hydroxide followed by biodegradation			
B BCF > 2000	80-100 *Oncorynchus mykiss* 100 calculated	No data 100 calculated	No data 445 calculated	No data 487calculated	No data 1579calculated
T long term NOEC < 10 µg/l STOT RE: Specific target organ toxicity after repeated exposure cat 1 or 2	NOEC of 1.12 µg/L *Daphnia magna* reproduction test STOT RE 1, H372	No data STOT RE 2, H373	No data STOT RE 2, H373	No data STOT RE 2, H373	No data STOT RE 2, H373

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According to the EU classification of phenlmercury acetate (T, R48 and STOT RE 1, H372) and of the other phenylmercury compounds (STOT RE 2), phenylmercury acetate, phenylmercury propionate, (2-ethylhexanoato) phenylmercury, phenylmercury octanoate and phenylmercury neodecanoate fulfil the T criterion in REACH Annex XIII.

All five phenylmercury compounds dissociate rapidly into phenylmercury cation and carboxylate anion followed by a rapid hydrolysis of phenylmercury to phenylmercury hydroxide. With phenylmercury as the common intermediate, it is considered likely that the propionate, octanoate, 2-ethylhexanoate and neodecanoate do not behave differently from the phenylmercury acetate with regard to biodegradation. Half-lives for phenylmercury acetate in waters, sediments and soils are below the persistency criterion (P).

The estimated BCFs for the five phenylmercury compounds in water with pH5 are between 100 and 1579 and the criterion for bioaccumulation (B) is not fulfilled.

The five phenylmercury compounds themselves are therefore not considered as PBT or vPvB substances.

Degradation/transformation products

	Methylmercury
P Half-life, fresh water > 40 d	Lower rate of demethylation than methylation under certain environmental conditions. Long half life (2 years) for elimination in organisms. The cycling of mercury means that the source for formation of methylmercury in the environment is always present, once released.
B BCF > 2000	8140 -85 700 in fish
T Long term NOEC < 10 µg/l Carcinogenic, mutagenic (category 1A or 1B), or toxic for reproduction category 1A, 1B, or 2); evidence on chronic toxicity	NOEC 0.26 Hg µg/L *Daphnia magna* reproduction test Repr. Cat 1; R61, Repr. Cat 3; R62 and T; R48/25

Fish appears to strongly accumulate methylmercury. Most of the methylmercury in fish tissue is covalently bound to protein sulfhydryl groups. This strong binding is the reason for a long half-life of about two years in biota and as a consequence methylmercury is biomagnified significantly through the food web. With BCF factors in fish in the range of 8140 up to 85700 methylmercury clearly fulfils the REACH Annex XIII criteria for bioaccumulation (B) and the criteria for very bioaccumulative (vB). The criteria for toxicity (T) with a NOEC of 0.26 µg/L for a *Daphnia magna* reproduction test and a provisionally agreed classification of methylmercury as Repr. Cat 1; R61, Repr. Cat 3; R62 and T; R48/25 is also fulfilled. Concerning the persistency (P) criteria the facts that demethylation occurs at a much lower rate than methylation under certain environmental conditions and that the biological half-life of methylmercury is high should be judged as of equivalent concern. As documented (B.4) the release and degradation of the phenylmercury compounds contributes to the pool of elemental and inorganic mercury which cannot be broken down to any harmless form. The cycling of mercury means that the source for formation of methylmercury in the environment is always present, once released. The measured environmental concentrations of mercury and methylmercury and the increasing trends of methylmercury levels in biota are of concern.

Overall, it is concluded that methylmercury is a PBT like substance or a substance of equivalent concern.

B.8.2 Emission characterisation

The main objective of the emission characterisation for a PBT/vPvB substance is to estimate the amounts of the substance released to the different environmental compartments during all activities and uses. If transformation/degradation products with PBT-properties are being generated, the substances themselves must be treated like PBT-substances with regard to emission estimation and exposure control. To this end, the exposures and emissions to humans and the environment should be minimized to the extent possible.
As a minimum, this applies if transformation/degradation products with the PBT/vPvB properties in amounts ≥ 0.1 % are being generated, or unless it is possible to estimate with sufficient certainty that the total amount of degradation/transformation products with PBT/vPvB properties generated by the substances do not exceed 1 t/y. Any release of the mercury compounds contributes to the mercury pool and consequently a potential for formation of significant quantities of methylmercury. Due to lack of data a quantification of the percentage of transformation/degradation products with PBT-like properties, i.e. methylmercury, could not be performed. However, considerations of the total volume, use pattern and emission pattern of the substances is of relevance in this context.

Information about manufacture and use of the substances is given in Section B 2. General information about release and exposure is given in Section B 9. Based on the information obtained it is estimated that around 75 – 150 tpa of phenylmercury compounds are manufactured for use in the production of phenylmercury catalysts in EU+EFTA, of which 40 – 85 tpa are exported. A substantial amount of phenylmercury compounds are manufactured exclusively for export (55 – 110 tpa). The estimated EU + EFTA consumption is approximately 36-70 tonnes (mainly phenylmercury neodecanoate), which corresponds to a total mercury content of approximately 16 – 31.3 tonnes/year, this includes a minor import.

The use of the catalysts is wide dispersive. The total number of companies applying the mercury-containing PU systems is not known but likely several thousands. Moreover, the mercury catalyst is incorporated into the polymer structure and remains in the final product. The mercury-based products are used both for the professional market and for consumer products. The life-cycle of the substances used in the EU+EFTA is estimated to lead to a release of 6.4 tpa of mercury to the environment (6.1 tpa to air) in 2008. This was estimated at around 4% of the estimated European emissions of mercury in 2005 and at around 7% of the reported emissions to air for EU-27 in 2008. Main releases are assumed to be from formulation and processing (large number of sites), service life and the waste phase. Once emitted, mercury enters the complex biogeochemical cycle. The formation of methylmercury under certain environmental conditions and subsequent biomagnification through food webs is of major concern.

According to the estimations a large amount of mercury (25 tpa) will accumulate in the landfills and apparently remain there. The long-term fate of mercury in the landfill is not known, evidently there is a potential for a release to the environment at a later stage (see also B.4.1.2.3 and B.9.5.3.2).

B.9 Exposure assessment

B.9.1 General discussion on releases and exposure

B.9.1.1 Summary of the existing legal requirements

No Community wide regulations exist for the import, manufacture, placing on the market or use of the phenylmercury substances for the production of polyurethane or articles containing the substances.

National policies and best practices in Europe going beyond EU legislation on mercury and/or mercury containing products exist in Denmark, Finland, Germany, Netherlands, Sweden, Spain, United Kingdom, Switzerland and Norway (Bio Intelligence Service, 2010). Only where general bans are implemented on the import, manufacture sale and/or use of mercury and mercury containing products (DK, NL, SE, CH, NO), phenylmercury substances for the production of polyurethane are regulated.

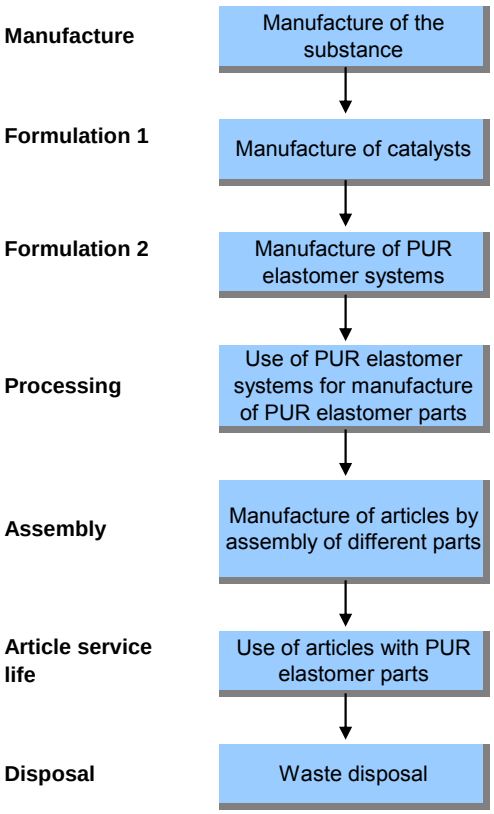
Some EU Member States have more stringent restrictions on the leaching limit values for mercury from landfills than EU acceptance criteria as defined in Council Decision 2003/33/EC and some Member States have recommendations on restriction of fish consumption going beyond recommendations from the European Food Safety Authority (EFSA) (Bio Intelligence Service, 2010). Such regulations are not considered to have substantial effects on the risks for mercury exposure from the production of polyurethane or articles containing the substances.

B.9.1.2 Summary of the effectiveness of the implemented operational conditions and risk management measures

Existing risk management measures, as presented in Section E, are not considered to reduce the risks of the mercury exposure from the use in polyurethane systems sufficiently.

B.9.1.3 General issues related to releases and exposure

The major life cycle stages for the use of the substance as catalyst in PUR elastomer systems are shown below:



The following environmental release categories (ERC) are considered relevant for description of the life cycle stages:

Table B-54 Environmental release categories (ERC) for the different life cycle stages

ERC Number	Name	Life cycle stage
ERC 1	Manufacture of substances	Production of the phenylmercury compounds
ERC2	Formulation of preparations	Formulation of catalyst by mixing of phenylmercury compounds with other constituents Formulation of one component of the two-component PU system by mixing the catalyst with otther constituent (mainly the polyol part)
ERC6d	Industrial use of process regulators for polymerisa-tion processes in produc-tion of resins, rubbers, polymers	Industrial use of PU two-components systems for processing of PU components
ERC8f	Wide dispersive outdoor use resulting in inclusion into or onto a matrix	Use of PU two-component adhesives, sealants and elastomers in non-industrial settings
ERC10a	Wide dispersive outdoor use of long-life articles and materials with low release	Use of PU automotive applications, ship fenders, conveyor belts, etc.
ERC11a	Wide dispersive indoor use of long-life articles and materials with low release	Use of PU flooring, rollers, coatings, etc.

The final articles have no intended release of the mercury compounds. Relevant article categories from the use descriptor system (ECHA, 2010d) are listed in Table B-55. The PU parts may be used in a large number of different article categories e.g. as a coating of one part of the article. Based on the available information it is not possible to point at specific article categories that account for the major part of the application of mercury catalysed PU.

Table B-55 Relevant article categories (AC) with no intended release

Article category (AC)	Description
AC 1-1	Passenger cars and motor cycles
AC 1-2	Other vehicles: Railway, aircraft, vessels, boats, trucks, and associated transport equipment
AC 2	Machinery, mechanical appliances, electrical/electronic articles
AC 3-1	Electrical and electronic products, e.g. computers, office equipment, video and audio recording, communication equipment
AC 3-3	Electrical and electronic products: Household appliances (white ware)
AC 7	1 Metal products: cutlery, cooking utensils, pots, pans,
AC 7	2 Metal products: toys
AC 7	3 Metal products: furniture
AC 10-2	Rubber products: flooring
AC 10-3	Rubber products: footwear
AC 10-4	Rubber products: toys
AC 10-5	Other general rubber products
AC 12-1	Constructional articles and building material: wall construction material ceramic, metal, plastic and wood construction material, insulating material (without indoor flooring)

Note: It is here assumed that the term "rubber" also includes synthetic rubber; otherwise the article categories for plastic products should be included instead.

Chemical forms

For the assessment of releases and the subsequent exposure it is relevant to distinguish between releases of different chemical forms:

- The compounds themselves.
- Elemental mercury from the breakdown of the compounds in processes or within preparations and articles.
- Other breakdown products from the breakdown of the compounds in processes or within preparations and articles.

Most available studies concern the releases of elemental mercury from paints and elastomer flooring containing phenylmercury acetate. No studies concerning the releases of phenylmercury neodecanoate or the other compounds from processes, preparations or articles have been identified.

Chemical forms released from articles

According to ATSDR (2008) the chemical literature is not clear about whether the mercury vapor from PMA or other mercury compounds found in floorings is elemental mercury vapor, or if it is the vapor form of the mercuric compound in the flooring. Because the Lumex Mercury Analyzer which has been used in analyzing mercury vapour in air in gymnasiums with mercury-catalyzed polyurethane flooring shows the presence of elemental mercury vapor

only, it is clear that PMA (or other mercuric compound) is slowly being converted to elemental mercury. However, it is not known if PMA in the floor is converted to elemental mercury prior to volatilizing, or if it is converted to elemental mercury in air. This question needs additional research according to ATSDR. If PMA is in vapor form in air, then the mercury concentrations in air that are reported understate the actual total mercury concentrations in air (ATSDR 2008).

The ATSDR toxicological profile for mercury (ATSDR, 1999) discusses different studies concerning releases from paints containing phenylmercury acetate (application of mercury containing paint most probably does not take place in the EU today). A case study reporting neurological effects in a boy after exposure to mercury vapour released from paint containing phenylmercury acetate was discussed under metallic mercury because the exposure was to metallic mercury vapours released from the paint (Aronow *et al*., 1990 as cited in ATSDR, 1999). In another study the authors reported that from 12 to 57% of the mercury in paint with phenylmercury acetate was emitted upon application as elemental mercury, with the highest emission rate within the first few hours after paint application (Tichenor and Guo, 1991 as cited in ATSDR, 1999). This use of phenylmercury resulted in the exposure of house painters and residents to elemental mercury vapours in homes where interior or exterior latex paint was applied (ATSDR, 1999).

The New Jersey Mercury Task Force states that several studies had indicated that when mercury-containing coatings and paints were applied, the painted surfaces released elemental mercury to the air (NJ MTF, 2002). The primary chemical species emitted from painted surfaces is according to the Task Force believed to be elemental, although the parent compound itself, phenylmercury acetate or a related substance, may be emitted as well. For estimating the temporal pattern of mercury releases from surfaces to which this paint was applied the Task Force applies, on the basis of the results of several studies, a half-life of the mercury in the paint of 1.5 year and a first-order exponential degradation model (NJ MTF, 2002).

Chemical forms of releases from waste incineration
In one process, waste incineration, the phenylmercury compounds are expected to be initially nearly 100% degraded. The mercury speciation in the flue gas will be dependent on the chemical composition of the incinerator flue gas and the temperature regime in the flue gas with elemental mercury, mercury oxide and mercury halides usually being the dominant forms.

Releases quantified as elemental mercury
Due to the limited data available on the chemical form of mercury released from processes and articles, the releases will for Tier 1 be quantified as elemental mercury.

B.9.2 Manufacturing

B.9.2.1 Occupational exposure

Inadequate information on occupational exposure related to manufacturing was available for this report.

B.9.2.2 Environmental release

Phenylmercury compounds and elemental mercury may be released by the manufacturing of the phenylmercury compounds and the catalysts.

Data on environmental releases has been provided by the major European manufacturer of the five phenylmercury compounds. Based on these data total environmental releases from the manufacturing of the compounds in the EU and EFTA have been estimated assuming that the emission factors are similar from all manufacturing processes.

Mercury emission to air is reported from one European manufacturer to take place from the reactor, the factory building and from the waste water treatment plant. The outlets are equipped with scrubbers for emission abatement. In 2008 the concentration in the outlet gas was measured at 0.05-0.08 mg/Nm3 (normalised m3). The emission factor for emission to air is estimated at 0.0016% of the total mercury used in the manufacturing process. Total mercury use in the EU+EFTA for manufacturing is in the range of 60-120 tonnes Hg/year. Total mercury emission to the atmosphere, using the maximum estimate of 120 tonnes mercury, is estimated at 1.92 kg/year. Only data on total mercury concentration have been reported. No data indicating the mercury speciation or the releases of the individual compounds have been available.

Mercury releases to waste water have been reported by one major manufacturer. The total mercury concentration in the waste water, after treatment within the company, was in 2008 for a single measured value measured at 20 mg/m3; of this 17.8 mg/m3 as dissolved mercury. This measured value in waste water is representative for measurements in 2008 according to manufacture. The emission factor can on the basis of the reported data be estimated at 0.00015%. The total releases from manufacturing processes in the EU+EFTA can on this basis be estimated at 0.2 kg/year. No further information on waste water treatment before discharge is available.

Ambient mercury concentrations at two sites just outside the factory building have been measured to be <0.015 μg/Nm^3 (normalised m^3) as particulate mercury and <0.2 μg/Nm^3 as gaseous mercury. For both parameters the concentration was below the detection limit.

From the U.S.A. it is reported that during the production of mercury compounds, emissions of mercury vapour and particulate mercury compounds may occur at the following sources: reactors, driers, filters, grinders, and transfer operations (U.S. EPA, 1997). However, no specific data were provided in the report for estimation of emission factors from the manufacturing process.

In addition, data are not numerous and were associated with some uncertainties. It could be notably noticed a conflict between the operational hours per year putted forward by manufacturer and the continuous process mentioned in monitoring documents, the absence of information on waste handling (filters, sludge...), as also monitoring values which were not checked against mass balance calculations. The default release factors proposed in R16 ECHA guidance (5% for air, 6% for water and 0.1% for soil) appear however too high. So both values are unrealistic but data are insufficient to calculate how high the underestimation is. Conclusion can thus only be that emissions from manufacture are higher than 0.0016% and 0.00015% to air and wastewater, respectively.

B.9.3 Use as catalyst in PU elastomer systems

B.9.3.1 General information

The major application of the phenylmercury compounds is as catalyst in polyurethane (PU) systems for CASE applications, in particular as elastomers, see B.2.2.

Releases to the environment and human exposure may primarily take place at the following stages:

- Formulation of PU systems (a mixture of 60-70% phenylmercury neodecanoate and 30-40% neodecanoic acid is typically added to the polyol part of the two-component system).

- Application of PU two-component systems (the polyol part with 0.2-0.8 % phenylmercury neodecanoate is mixed with the isocyanate part to form the final component).

- Article service life (the PU parts typically contain 0.1-0.6% phenylmercury neodecanoate but the concentration range may also be wider, cf. Section B.2.2).

- Waste life.

For some applications, the PU component (e.g. a wheel) may be assembled with other components to form an article (e.g. some roller skates), but the releases and human exposure by this lifecycle stage (assembling) is considered to be small compared to the other stages and not included in the assessment.

Formulation of the PU elastomer system: Work practices

Work practices involved during the formulation of the PU systems have been described by two contacted formulators of the PU systems in relatively small scale (indicated as A and B). It has not been possible to obtain a detailed description for large-scale formulators and large-scale applications.

A: A small quantity of liquid mercury catalyst is added to a polymer system in open batch mixers with local exhaust ventilation. The process is split into three main stages, weighing out of raw materials, batch manufacture and filling. Mixing takes place at room temperature and at low speeds.

B: Formulation is carried out at the laboratory bench according to general laboratory practices, using small containers of mercury catalyst. All the formulation work consists of mixing a number of liquids to give a polyol blend. These are then reacted with an isocyanate to give the finished polyurethane system. Workers wear at least the minimum required PPE (gloves, eye protection, coats or coveralls). Maximum of 0.5 grams per formulation of the catalyst is added to the formulation with a syringe or dropper. The amounts of catalysts used at this stage of the formulation process are a. After use, the catalyst container is resealed and the syringe or dropper is disposed of in a specially designated container. At this point in the formulation process if any leaks or spills occur they will be fully contained at the laboratory bench. Contaminated containers, clothes, absorbents and gloves will be disposed of in the reserved container.

By the application (processing) of the PU system the two components are mixed together and poured into a mould or applied by other means. Different processes are applied and some examples provided by formulators of the PU systems are given in B.2.2.

B.9.3.2 Exposure estimation

B.9.3.2.1 Workers exposure

No data on actual measurements of occupational exposure and release to the environment have been obtained from the contacted formulator companies A and B, presented in Section B.9.3.1. As concern occupational exposure, it should be noted that the main concern of the users is the isocyanate part which takes up a major part of the mixture and is classified as toxic by inhalation. Exposure to mercury from the processes seems not to be a concern for the users. The applied personal protection equipment will mainly be governed by the legislative requirements for working with isocyanates, such as ventilation and the use of personal protcetive equipment (PPE). According to the formulators, there are a number of statutory requirements regarding the use of isocyanates in the workplace.

The responding companies in general consider the releases of mercury to the environment by the application of the PU systems to be negligible.

Some of the users of the PU systems store and react them in dedicated rooms, fume cupboards and glove-boxes. Again the containment and removal of the isocyanate vapour would also apply to any mercury vapour. The exhaust seems in general not to be equipped with mercury-specific filters.

According to contacted companies workers usually do not wear respiratory protection.

Use of PU elastomer system: Exposure scenario
No exposure scenarios covering the formulation and application (processing) of the mercury-containing PU systems have been obtained from the formulators or suppliers of the systems.

Tier 1 occupational exposure estimation
In the following an exposure scenario for an open application of the PU systems for casting of PU parts (use of PU systems) is set up, and a Tier 1 occupational exposure estimation is performed using ECETOC TRA Tool version 2.

The most likely occupational exposure route would be by inhalation. The worker might be exposed to the mercury catalyst phenylmercury neodecanoate evaporated from the raw materials or to degradation products, such as mercury vapour.

Input
In the process assessed it is assumed that the two components of the PU system are mixed by hand in an open container in a ventilated area at room temperature (20 ºC). No exhaust is applied. It is assumed that the PU is used for moulding.

For the Tier 1 estimation it is of high importance in which form the mercury is released and which vapour pressure is applied for the estimates. The workers may be exposed by inhalation of evaporated phenylmercury compounds, elemental mercury or other degradation products.

According to the REACH guidelines for occupational exposure estimation personal protection equipment (PPE) is generally not considered for the Tier 1 estimate, even if PPE is used in real-life (ECHA, 2010e).

In the exposure scenario it is assumed that the vapour pressure of the pure substance is the same when it is diluted in a solvent.

The parameters used for the estimation is shown in Table B-56

The ECETOC TRA tool uses the vapour pressure as a surrogate for fugacity as defined in an availability banding for an initial assessment. The fugacity and the process category together with the other input parameters define selection of default exposure prediction values for the estimation.

As no vapour pressure is available for the phenylmercury neodecanoate the vapour pressure of 0.0007999 Pa for phenylmercury acetate is used. In the ECETOC TRA tool this corresponds to a low fugacity.

Output
When using activity durations of <15 minutes and 1-4 hours, respectively, the following inhalation exposure estimates are obtained:

- Duration 1-4 hours: 0.084 mg/m^3 (0.05 mg/m^3 Hg)
- Duration <15 minutes: 0.014 mg/m^3 (0.008 mg/m^3 Hg)

Table B-56 Parameters used for Tier 1 occupational exposure estimation using ECETOC TRA tool

Physical state of the substance	Liquid
Physical state of the product handled	Liquid (until it is cured)
Vapour pressure	$6.00x10^{-6}$ mm Hg (at 20° C) (ChemID, 2009) corresponding to 0.0007999 Pa. Value for phenylmercury acetate – the value may be used in absence of value phenylmercury neodecanoate The vapour pressure of the catalyst with phenylmercury neodecanoate is reported to be < 5 mm Hg
The concentration of the substance in the preparation	<1%. The actual concentration in the total mixture is in the range of 0.05-0.5 % (after mixing of the two components)
Process	5- mixing and blending in batch processes (multistage nad/or significant contact.
Activity type	Industrial
Duration of activity	For the Tier 1 estimation it is assumed that the duration is <15 minutes or 1-4 hours.
Indoors/outdoors	Indoors
Ventilation present	For the Tier 1 estimation it is assumed that no ventilation is present
Efficiency of respiratory protection	For the Tier 1 estimation it is assumed that the mixing takes place without respiratory proection

Release from articles: Exposure scenario

Beaulieu *et al*. (2008) reports mercury level in air, as well as in blood and urine from workers during controlled abatement of an old mercury-containing gymnasium flooring. Increased levels of mercury in blood are thought to be indicative of recent exposures to mercury vapor, while increases of mercury in urine are thought to be indicative of long-term exposures. No measurable concentrations of mercury were found in the urine of workers, and only insignificant increases of mercury were found in the blood. The levels in air are reported in Section B.9.3.2.2.

B.9.3.2.2 Consumer exposure

Elemental mercury or phenylmercury compounds are not released intentionally from articles with phenylmercury compounds.

The major exposure of consumers due to the use of phenylmercury compounds in polyurethanes is expected to be exposure to elemental mercury and mercury compounds released during the service life of articles and exposure to mercury compounds via the environment (see B.9.3.2.3).

Exposure of humans to mercury catalysts in articles may take place by different routes:

- Inhalation of evaporated phenylmercury compounds, elemental mercury or other degradation products.
- Dermal contact to phenylmercury compounds, elemental mercury or other degradation products leached from the articles.

- Ingestion of dust particles with phenylmercury compounds or other degradation products formed by abrasion of articles.
- Exposure to mercury from articles put in the mouth intentionally is considered negligible.

Most probably a large number of different articles may each lead to minor exposure of the general population. Examples of articles that may lead to exposure of consumers are the following:

- Flooring.
- Elastomer coatings e.g. for leather finishing, textile and fibre treatment or coating of computer parts.
- Rollers e.g. on roller skates and swivel chairs.

Release and measured indoor air concentrations

Actual investigations of mercury release from articles have only been identified for PU elastomer flooring. PU flooring with mercury catalysts has previously been widely used in school gyms and sport arenas in the U.S.A. (and probably also in Europe). Polyurethane flooring is widely applied in the EU today, but different non-mercury catalysts seem to be used for this application, and no information on the actual use of mercury catalysts for flooring have been obtained. According to a consulted company active on the European market, mercury-containing PU floors were produced in Europe and exported, but it is also possible that it was marketed in Europe. This could not be further confirmed, however (pers. comm.).

Use of phenylmercury compounds in flooring may be considered as a worst case exposure scenario. The floors have large surface area from which the mercury and mercury compounds can be released. There is a potential for three types of exposure to heavy metals from the gym floorings: inhalation of vapour or dust particulates from the flooring, dermal contact with the flooring, and ingestion of residues or dust particulates from the flooring (ATSDR, 2008). An investigation of mercury releases from mercury-containing Tartan flooring showed that about 98% of the mercury in the air was in the vapour phase and about 2% bound to particles (Beaulieu *et al*., 2008).

Both EPA and IPCS have determined a Reference Concentration (RfC) of mercury vapour for the general population. Based on the LOAEL for effect on the central nervous system (occupational exposure data) the EPA determined a RfC of 300 ng/m^3 (US EPA, 1997). A RfC is an estimate of a continuous inhalation exposure concentration to people (including sensitive subgroups) that is likely to be without risk of deleterious effects during a lifetime.The US ATSDR established a minimum risk level (MRL) of 200 ng/m^3, also based on the occupational data. Using the ATSDR document as the source document, and complementing the information with further studies IPCS identified 200 ng/m^3 as a guidance maximum value for long-term inhalation (WHO, 2003).

To our knowledge flooring is the only application in articles where actual measurements of exposure exist. Studies where levels of mercury vapour from floors have been measured are described below. As far as we know the concentration of PMA compounds in these floors (up to 0.1%) are in the same range as in the articles which is now on the market and which will be affected by the proposed restriction.

According to an investigation by the Minnesota Department of Health (U.S.A.), some PU elastomer flooring manufactured from about 1960 through at least 1980 contained up to 0.1% mercury as PMA or other organo-mercuric salts that were used as catalysts (Reiner 2005, as cited by ATSDR 2006). This concentration is similar to the concentration in PU elastomers applied for different products today.

According to ATSDR (2008) the chemical literature is not clear about whether the mercury vapor from PMA or other mercury compounds found in floorings is elemental mercury vapor, or if it is the vapor form of the mercuric compound in the flooring. Because the Lumex Mercury Analyzer shows the presence of elemental mercury vapor only, it is clear that PMA (or other mercuric compound) is slowly being converted to elemental mercury. However, it is not known if PMA in the floor is converted to elemental mercury prior to volatilizing, or if it is converted to elemental mercury in air. This question needs additional research according to ATSDR. If PMA is in vapor form in air, then the mercury concentrations in air that are reported in this document understate the actual total mercury concentrations in air.

Environmental Health Information from Minnesota Department of Health states that when new, these floors contained up to 0.1% mercury, but as the floors age, the mercury content slowly decreases, so levels in floors that are decades old can be considerably less than 0.1% (MDH, 2008a). No documentation on the decrease in the mercury content is provided.

Four publications with results from sampling of air from gymnasiums have been identified (ATSDR, 2003; ATSDR, 2006; ATSDR, 2008, and Beaulieu *et al*., 2008). Only one was published in a peer reviewed journal, and describes exposure and biomonitoring for abatement workers (Beaulieu *et al*. 2008). The others were investigations initiated due to health concern for children, students and faculty from mercury-containing polyurethane floors in schools. In all the reports mercury levels were determined by Lumex Mercury Analyzer. Beaulieu *et al*. also applied sampling onto carulite tubes (average ~8 hours) followed by analysis using NIOSH Method 6009, Mercury. The Lumex Mercury Analyzer is a portable instrument for in-situ measurement of elemental mercury vapour. As it measures the elemental mercury concentration every second, it has the limitations of any direct-reading instrumentthat it gives a snapshot of the exposure in a very short time interval. It does not determine fluxes in the exposure and it is thus not an instrument to achieve 8 hours time weighted average values or to determine continuous exposure. So even if the measurements were done in or close to the breathing zone, the relevance to compare the results with MRL, Rfc or DNELs have been questioned in the public consultation. Still we consider the reports to present a “worst case” situation, especially when the ventilation in the gymnasiums is switched off. It should however be recognised that since mercury-containing PU-floorings mainly were installed from about 1960 through at least 1980, exposures to new floorings may be assumed to have been higher than those measured for old floorings, see chapter B 9.5.2. In the reports comparison to EPA RfC is given. This RfC is adjusted to 24 hours, 7 days per week exposure. For comparison with relevant DNELs see chapter B.10 and Appendix 1 (ATSDR, 2008).

In a study from Minnesota (U.S.A.), ambient mercury vapour concentrations in school gyms ranged from 130 to 2,900 ng/m^3 (30 sec Lumex results), and in 5 of 6 gyms the concentration was above the RfC set by the US EPA (300 ng/m^3) (ATSDR, 2006). The highest values (1369 and 2900 ng/m3) were measured when the ventilation was not running. Most of the samples were taken in summer, but the highest concentrations were sampled in April (2900) and October (1369). Ventilation running reduced mercury vapour concentration by 77 % in one

school. The study did not investigate whether mercury can be rubbed off of the surface of the floorings or if there is mercury in dust on the floors.

In another study, mercury vapour concentrations were measured using Lumex Mercury Analyzer on four different occasions in May and June prior to covering the mercury containing Tartan floor with a new surface in a university in Minnesota. Air concentrations of mercury were in the range of 323 to 2,699 ng/m^3. The highest levels (typically > 2000 ng/m^3) were found when ventilation fans were off and doors and windows were closed (ATSDR, 2008).

An investigation of mercury in bulk flooring material and mercury vapour in air was conducted in nine schools in Idaho (U.S.A) in the spring of 2006. The results showed that in a high school with two exposed Tartan brand flexible gymnasium floors and an additional floor encased with a wooden overlay floor, mercury levels in air were about 500 ng/m^3 (Ohio-Lumex instrument), or about 200 ng/m^3 (by sampling on carulite tubes ~8 hours and analysed using NIOSH Method 6009). These mercury vapour concentrations were about 20–50 times the concentrations of outside ambient air (Beaulieu *et al*., 2008).

The air concentrations will depend on the temperature, with higher emission rates at higher temperatures, and the ventilation of the rooms. Model calculations of mercury vapour concentrations in a gymnasium with mercury-containing floor showed seasonal variation at normal ventilation between 1,200 and 3,500 ng/m^3 (MDH, 2008a). With warm weather ventilation during summer, the concentration dropped to about 300 ng/m^3 (MDH, 2008a).

Table B-57 Long term exposure concentrations to consumers

Routes of exposure	Measured exposure concentrations		Explanation / source of measured data
	value	unit	
Oral exposure	Not data found		
Dermal exposure	Not data found		
Inhalation exposure	323-2699	ng/m^3	Air concentration measured as mercury vapour in a gymnasium in Minnesota with a mercury containing polymer floor (containing organic salts such as PMA or phenyl mercuric neodecanoate) ATSDR (2008).
	130-2900	ng/m^3	Air concentration measured as mercury vapour in a gymnasium in Minnesota with a mercury containing polymer floor (containing organic salts such as PMA or phenyl mercuric neodecanoate) ATSDR (2006).
	≤500	ng/m^3	Air concentration measured as mercury vapour in nine schools in Idaho (U.S.A) in the spring of 2006. (Beaulieu *et al*., 2008)
	n.d. -1430	ng/m^3	Air concentration measured as mercury vapour in four gymnasiums in Ohio with a mercury containing polymer floor (containing organic salts such as PMA or phenyl mercuric neodecanoate) ATSDR (2003).

In an investigation in Ohio, tests showed that five out of nine 3M Tartan Brand flooring should be considered hazardous waste as a material leaching test showed a concentration above 0.2 milligrams per litre (mg/l) (ATSDR, 2003). The results indicate that exposure by dermal contact may take place, but this exposure is considered insignificant compared to the exposure by inhalation. Using the Lumex Mercury Analyzer mercury vapour concentrations

in the indoor air of all schools were measured from non-detectable levels to 1430 ng/m^3 in the breathing zone.

Compared to the exposure to mercury emitted from flooring, exposure from other applications is considered to be low due to the relatively small surfaces from which the mercury can be emitted. However, most probably a large number of different articles may each lead to minor exposure of the general population. Some products, e.g. some adhesives and some moulding products are to a limited degree processed by consumers.

Wear and tear of surfaces may lead to increased emissions as mercury may be released from the particles and from the part of the surface which is exposed by the abrasion. High levels of abrasion may in particular be expected for some out-door uses e.g. shoe soles and roller skates rollers (discussed under B9.3.2), but these out-door applications are not considered to lead to significant direct human exposure. Also in some in-door applications high levels of abrasion may be expected, e.g. in rollers on swivel chairs. A theoretical quantitative estimation of possible air concentration of PMA in a bedroom from wheels on a swivel chair has been made. These data are presented in Appendix 1.

B.9.3.2.3 Indirect exposure of humans via the environment

Mercury released to the environment from the application of phenylmercury compounds contributes to elevated levels of mercury found in the environment and thereby contributes to the exposure of humans to mercury via the environment.

The phenylmercury compounds are degraded to hazardous degradation products, i.e. inorganic mercury compounds and elemental mercury, which can be transformed to methylmercury. Mercury and methylmercury may be generated from others sources than phenylmerucry compounds. For the phenylmercury compounds sufficient information is not available to make a quantitative risk assessment of the possible exposure level of man via the environment.

The questions regarding the exposure of man via the environment to mercury released from PU catalysts in articles, are quite similar to the questions regarding exposure to mercury via the environment from the use of dental amalgam addressed by the Scientific Committee on Health and Environmental Risks (SCHER) in its opinion on the environmental risks and indirect health effects of mercury in dental amalgam (SCHER, 2008). According to the committee this type of risk assessment requires, next to extensive general information on the effects to humans and (various) environmental species, more detailed information on possible regional-specific differences in the use, release and fate of mercury originating from specific uses. Thus a quantitative and causal relationship as regards the contribution from the release and degradation of the phenylmercury compounds to exposure estimates via the environment cannot be made. It should be noted that the use of mercury in catalysts for PU gives rise to a much wider range of emission sources than the use of dental amalgam.

The amounts of phenylmercury compounds released into the environment, calculated as mercury, may be compared with information on the overall emission of inorganic mercury. It is evident that the life-cycle of the phenylmercury compounds leads to a significant release of mercury to the environment (mainly to air). The life-cycle of the substances used in the EU+EFTA is estimated to lead to a release of 6.4 tpa of mercury to the environment (6.1 tpa to air) in 2008. This was estimated at around 4% of the estimated European emissions of

mercury in 2005 and at around 7% of the reported emissions to air for EU-27 in 2008. Once emitted, mercury enters the complex biogeochemical cycle. Mercury is present in fish and seafood products largely as methylmercury, and fish is a useful indicator of human exposure. Food sources other than fish and seafood products may contain mercury, but mostly in the form of inorganic mercury (EFSA, 2004).

General information about exposure of man via the environment (mainly from fish and seafood products) is given in Appendix 1, 3.1.2)

B.9.4 Other sources (for example natural sources)

No data on formation of the five compounds in the natural environment have been found.

B.9.5 Estimate of emissions

These calculations only include emissions related to manufacture and products produced in the EU. Emissions in the EU from imported articles and emissions outside the EU from exported articles are not included.

B.9.5.1 Formulation and processing

No actual data on the releases of the substances or elemental mercury from formulation (i.e. formulation of the one component of the two-component PU system by mixing the catalyst with other constituent (mainly the polyol part)) or processing (application of the two-component system) has been available. While formulation probably takes place by 50 to several hundred companies, processing may take place by hundreds to thousands of companies. Some products, e.g. some adhesives and some moulding products are to a limited degree processed by consumers.

The guidance on Environmental Exposure Estimation (ECHA, 2008d) states that if the uses are covered by branch-specific OECD and EU emission scenario documents these may be used instead of the default environmental release categories (ERC).

Emission factors for the process can be derived from default emission factors provided in the TGD (TGD 2003) and the Emission Scenario Document for Plastic Additives (OECD, 2004).

By the formulation of the PU system, the mercury containing catalyst is mixed with other constituents to make one of the components of the two-component system. One of the applied catalysts with phenylmercury neodecanoate is described as "clear yellow, viscous liquid with a mild odor" (Vertellus 2009a). The boiling point of the catalyst is 200 ºC and the vapour pressure < 5 mm Hg at 20 ºC (<665 Pa). The catalyst is insoluble in water. According to industry, in general the processes do not involve the use of water, e.g. for cleaning of cured components.
It is assumed that other catalysts with phenylmercury neodecanoate have similar properties.

The TGD applies a default emission factor for IC = 11: Polymers Industry type II Catalysts (UC 43 process regulators), of 0 for both dry and wet formulation processes if the vapour pressure of the catalyst is <1 Pa. For releases to waste water the default emission factor is 0.0005 for "wet" processes if the water solubility is < 10 mg/l.

For processing of thermosetting resins the default emission factors for curing agents and cross linking agents are:
Air: 0.075 (agents with a vapour pressure <100 Pa)
Waste water: 0.00005
Soil: 0.00001

The Emission Scenario Document (ESD) for Plastic Additives applies for liquid curing agents the following default emission factors (OECD 2004):

Raw materials handling
Air: 0
Waste water: 0.0001

Compounding
Air: 0.00005
Waste water: 0.00005

It is in the emission scenario document assumed that initial losses will be to atmosphere, vapours will condense to some extent, resulting in losses to both solid waste and aqueous washings. It is assumed that the volatilisation loss will condense to some extent and eventually be released 50% to air and 50% to waste water.

The emission scenario document assumes that the losses by conversion (application), service life and disposal are 0. Accordingly, the emission factors

Fconversion = Fservice life = Fdisposal = zero (material destroyed) for both air and water."

The reasoning for this is as follows: "Once in the plastic, they would begin to decompose as fabrication commences and would be expected to be fully destroyed once fabrication is complete."

Concerning the mercury catalysts it might be correct that they are decomposed, however the decomposition products would be other mercury compounds or elemental mercury, and these might be released into the environment. Furthermore, the assumption that processing of PU typically takes place in totally enclosed systems cannot be concluded based on the information obtained from industry. In small-scale production the application of Hg-containing catalysts either takes place in a well-ventilated area or under a fume hood. Some of the users of the PU systems state that they store and react them in dedicated rooms, fume cupboards and glove-boxes and that containment and removal of the isocyanate vapour would do likewise for any mercury vapour. According to the information obtained exhaust systems are not equipped with specific mercury filters. It must therefore be expected that the major part of mercury released from the process is released to the surroundings by the ventilation air. No information about use of exhaust abatement systems from large-scale processing has been provided by industry.

For non-industrial processes the components may be mixed and filled into a joint (sealants) or smeared on surfaces (adhesives).

Based on the above, the default emission factors from the TGD are considered the most relevant to apply for the estimation of releases of phenylmercury compounds, because they includes emissions from processing. The TGD states regarding the default emission factors: "The emission factors were established by means of expert judgement and tended to the worst-case situation" (p. 217).” The actual emission factors may be different than those suggested by the TGD, but due to the lack of sufficient information, these are used as the best estimate.

The total emission from raw material handling, formulation and processing will be estimated using the following emission factors:

Air:	0.075
Waste water:	0.0006 (0.0005 + 0.00005)
Soil:	0.00001

With a total tonnage of 31.3 tonnes mercury in 2008 the emission is estimated at:

Air:	2.35 tonnes Hg/year
Waste water:	0.02 tonnes Hg/year
Soil:	Negligible

With a total release from these life cycle stages of about 2.4 tonnes Hg/year it is estimated that approximately 28.9 tonnes Hg/year ends up in the articles.

B.9.5.2 Service life

As described in Section B.9.3.1 mercury will be released from mercury-containing PU during service life. No data has been available on the total amount released during the entire service life.

The available data on releases from PU flooring may be used to indicate whether the releases during service life can be significant. The releases will probably be strongly dependent on whether part of the surface is removed by wear and tear. In an investigation from Minnesota it was noted that a basketball court with mercury-containing polyurethane floor had noticeable wearing (discoloration) of the floor under all baskets. This indicated that at least from this application the releases during service life can be significant.

Releases to air

In a number of studies in the U.S.A. (discussed above) mercury concentrations in gyms with mercury-containing flooring were measured.

ATSDR, 2008, report mercury vapor concentrations in a gym with mercury-containing PU-floor measured under different environmental conditions. Analytical and emissions data from small chunks of flooring had also been collected and were used to develop floor emissions. According to this report Hg-emissions from floors appear to be temperature dependent with emissions likely to double for every increase of about 5 degrees Celsius in air temperature. Therefore, emission rates may have strong seasonal-dependence. The half-life of mercury in the flooring was calculated to be about 16 years. Emissions from the gymnasium floors have likely occurred since the flooring was installed in the early 1980’s.

In accordance with this, the Environmental Health Information from Minnesota Department of Health states that when new, these floors contained up to 0.1% mercury, but as the floors age, the mercury content slowly decreases, so levels in floors which are decades old can be considerably less than 0.1% (MDH, 2008a).

Emissions during service life can be calculated based on the half life $T_{1/2}$ of 16 years for mercury in PU floorings as determined by ATSDR (2008). With a service life of 5 years, 19.5% of the mercury is likely to be released from PU floorings. Assuming a service life of 10 years, 35.2% of the mercury in PU floorings would be released into the air.

The total releases during service life will depend on the surface to volume ratio and the service lifetime of the articles. PU-floors have a very high surface to volume ratio and the release estimated for PU- floors may therefore be in the upper end of the range compared with other PU-articles. PU elastomers may have a very long technical lifetime as indicated by the fact that many floors laid or poured sometime between the 1960s and the mid 1990s still exist today.

As the releases probably is also highly dependent on wear and tear, which increase the exposed surface, it must be expected that the percentage released during the service life from some applications e.g. shoe soles and roller skates rollers can be comparable with the percentage released from floors, whereas it may be significantly lower from other applications e.g. rollers in machinery and use in electronic encapsulation.

Based on the scarce data available it will here be assumed that an average of about 9-10 % of the mercury content is released to the air as elemental mercury or mercury compounds during the entire service life.

Releases to waste water

In an investigation in Ohio, tests showed that five out of nine 3M Tartan Brand flooring should be considered hazardous waste as a material leaching test showed a concentration above 0.2 milligrams mercury per litre (mg/l) (ATSDR, 2003).

From a formulator of PU systems test data for two of the mercury catalyst containing products has been obtained. The catalysts were independently tested back in 1987 by Enesco in the US. They tested for mercury leaching in accordance with the EPA 7471 method. The test involved a surface area to volume ratio of 1:5 and it was a 30 day soak test. The leaching measured was 1.6, 1.8 and 1.9 mg/l at 13, 21 and 32ºC respectively for one of the catalysts, and 0.49, 0.48 and 0.48 mg/l of the other catalyst at the same temperatures.

Releases of mercury to waste water may take place when washing the articles e.g. flooring or coated surfaces. For plasticisers used in flooring it is demonstrated that the abrasive releases are significantly higher than the leaching. For the plasticiser DEHP in flooring the abrasive releases to waste water are for example estimated at about 0.15% per year (COWI, 2009) corresponding to about 3% over a 20 years service life that will end up in waste water. For some applications e.g. shoe soles and roller skates rollers, as mentioned above, the abrasive releases may quite well be higher than the releases from floors, whereas for others the releases will be insignificant. On an average the total life-time emission factor could likely be in the range of 0.5% and 5%. In the absence of actual emission factors an average factor of 1% for all applications will be applied.

Direct release to aquatic environments
For some sub-sea and maritime applications where the PU may be used for corrosion protection, pipe jointing, non-skid surfaces, fenders etc. the mercury may be released directly to the seawater and this has been the background for some of the development of alternatives for sub-sea applications (IFS, 2007). No data on the direct releases to the sea has been available. Although the releases may be significant for the products used sub-sea, the total quantity is probably low, and the direct releases from sub-sea and maritime applications have not been quantified.

Total service life release
The service life release of total mercury from the articles put into use today, projected on one year assuming steady state consumption, can on the basis of the calculations above be estimated at:

Air: 2.75 tonnes Hg/year
Waste water: 0.26 tonnes Hg/year

B.9.5.3 Waste handling

Waste from formulation and processing
Work practices involved during the formulation of the PU systems have been described by two contacted formulators of the PU systems in relatively small scale (indicated as A and B). It has not been possible to obtain a detailed description for large-scale formulators and large-scale applications (see B.9.3.1). One formulator provided no information concerning waste handling.The other formulator stated that all mercury containing waste is disposed of in a designated container. This is for both laboratory generated waste and waste derived from production of the polyols. The designated container is emptied when necessary and its contents transferred to a separate container for consolidation. The consolidated waste is then disposed via licensed waste brokers able to accept mercury contaminated materials. Mercury contaminated waste production from the specific company is about 10 kg per year. This consists mainly of contaminated droppers and cleaning wipes with some single use containers.

According to information from a supplier most customers will react any excess material to give a solid polymer before disposing it of as waste. Waste may further be generated from raw materials exceeding the shelf life of the raw materials, but according to suppliers, customers try to eliminate the accumulation of time expired material which has the associated costs of disposal. One contacted formulator recommends their customers to use a licensed broker or contractor, whereas another supplier indicates that the reacted PU can be disposed of as regular waste. They report that ultimately the waste will go to landfill or incineration. One of the contacted companies has estimated that on average 5% of the raw materials ends up in waste from the application.

In accordance with the guidelines for estimation of exposure from waste life stage (ECHA, 2008e), a steady state is assumed i.e. the amount of the substance entering into the waste life stage corresponds to the actual consumption subtracted the releases by application and during article service life.

Waste from service life (articles)
The present mercury content of catalysts ending up in articles in EU + EFTA countries, as described in previous sections, is estimated at approximately 28.9 tonnes total mercury per year. A total of approximately 3.0 tonnes mercury/year is estimated to be released by application of articles and the total mercury content of articles entering into the waste stream is therefore estimated at 25.9 tonnes mercury per year.

Mercury containing articles and waste from the application of PU systems may be disposed of as follows:

- **Hazardous waste incineration and landfilling**: A small part, originating as waste from the application of the mercury-containing PU, may be disposed of as hazardous waste, but this part is assumed to be very small and has not been assessed separately.

  Mercury catalysed PU materials will typically contain the mercury compounds in concentrations in the range of 0.1-0.5%. In this concentration range, the waste of these materials would be classified hazardous according to the hazardous waste directive if the substances were classified very toxic, carcinogenic or mutagenic (EC, 2000). The phenylmercury compounds are in this concentration range not classified toxic, carcinogenic or mutagenic (see Section B1.3) and the waste materials are consequently not classified hazardous. Elemental mercury is classified very toxic (T+; R26) but the content of elemental mercury in the materials are considered to be below 0.1%. Waste of the catalyst product used for the formulation of the PU systems is classified hazardous, but the quantity of such waste is considered to be small.

  In the U.S.A. the mercury containing materials shall be disposed of as hazardous waste dependent on the mercury content of the material and the mercury leaching rate (MPCA, 2008). In an investigation in Ohio, tests showed that five out of nine 3M Tartan Brand flooring should be considered hazardous waste as a material leaching test showed a concentration above 0.2 milligrams per liter (mg/l) (ATSDR, 2003).

- **Recycling**: Polyurethanes are two-component systems that irreversible cure by the application (thermosets) and PU can, unlike thermoplastics like PVC or polyolefins, not be recycled. It is assumed that no recycling of PU takes place. Polyurethane elastomers, coatings, sealants and adhesives may follow metal parts that are disposed of for recycling e.g. in secondary steel or aluminium plants. The PU will generally be combusted by the recycling process and the mercury will be evaporated and ends up in the flue gas from the process. The percentage of the mercury that ultimately is released to the atmosphere will depend on the actual air pollution abatement system. The actual amounts of mercury-containing PU disposed of with metal for recycling is not known, but it is assumed to be a very small part and no specific estimates have been done for this disposal route.

- **Municipal solid waste incineration** and **landfilling**: It is assessed that the major part of articles with mercury containing PU ultimately ends up in the municipal solid waste stream for (municipal solid waste) incineration or landfilling.

The total quantity of municipal solid waste generated in the EU27 around 2005 was by the European Topic Centre on Resource and Waste Management estimated at 254million tonnes

(Skovgaard *et al*., 2008). Of the municipal solid waste generated in 2005approx. 45% was directed to landfills, 18% was directed to incineration while the remaining 37% was recycled or recovered (Skovgaard *et al*., 2007). However, as recycling/recovery activities addressing PU elastomers does in general not take place, it is estimated that in reality nearly all PU elastomers present in end-products will ultimately be directed to either landfills or incineration. Thus, the figures presented above are here adjusted to 71% to landfills, 29% to incineration and 0% to recycling. Some elastomers e.g. used in cars may follow the steel scrap to remelting and result in mercury emissions from secondary steel production, but the amount are assumed to be small and has not been addressed specifically.

Assuming that 71% is directed to landfills and 29% to incineration, the 25.9 tonnes/year ending in the municipal solid waste stream will result in 18.4 tonnes/year directed to landfills and 7.5 tonnes/year directed to municipal solid waste incineration.

B.9.5.3.1 Incineration

By the incineration process the henylmercury compounds are expected to be broken down completely to elemental mercury. The emission will depend on the actual abatement systems applied. Due to the nature of mercury, traditionally a significant part of the mercury has passed the emission abatement systems. With modern incinerators, equipped with specific abatement systems for control of dioxin/furans and mercury, the mercury emission factor is typically in the range of 10-20%.

According to the guidance for estimation of exposure from waste life stage (ECHA, 2008e), the mercury emission factors at tier 1 for emission to air after abatement (controlled emission) hazardous waste incineration, municipal waste incineration and co-incineration in industrial combustion plants was 0.1[10]. The emission factor was calculated from information available in EU Reference Document on Best Available Techniques (BAT). Further, it was in the guidance estimated that on average 0.02% of the mercury ends up in waste water after abatement.

Assuming that 29% of the mercury catalyst in the municipal solid waste stream is incinerated and that 10% of the mercury in the incinerated waste is emitted to air, the total emission to air from municipal solid waste incineration can be estimated at 0.75 tonnes Hg/year.

The emission factor of 10% represents the BAT, whereas the actual average emission from European incineration plants probably is significantly higher. In a recent inventory of product related emission in the EU, Kindbom and Munthe (2007) apply an emission factor of 50% for mercury emission from waste incinerators. Kindbom and Munthe (2007) estimate that about 20 tonnes mercury per year in waste is directed to waste incineration resulting in an emission of about 10 tonnes per year (best estimate). Based on the UN statistics it was in the study assumed that approximately 20% of the municipal solid waste was incinerated in the EU. The emission from waste incineration represented a major part of the product related emissions in

[10] According to the revised Guidance Chapter R.18, version 2 ECHA, 2010c : Estimation of exposure from waste life stage; a factor 0.05 is assumed for mercury. However, it is noted that "This factor can be used up to a mercury concentrations in the waste input of about 7 mg/kg (dry substance, 20% exemplary waste water content). Higher mercury concentrations would exceed the emission limit value of 0.05 mg/m^3 of the Waste Incineration Directive. Such waste fractions would be directed to underground disposal instead of thermal treatment." The mercury concentration in waste containing the PU components with phenylmercury catalysts may be significantly higher.

the EU, which was estimated at a total of 12-23 tonnes/year. The use of mercury in PU was not included in the estimate of mercury directed to waste incineration as this use was not described at the time of the analysis.

Using an emission factor of 0.02% to waste water the total emission to waste water from waste incineration can be estimated at about 0.001 tonnes Hg/year. In fact, the amount ending up in waste water depends on the actual abatement system, and for some systems no waste water is generated, but the average will be used for the estimations here.

Mercury is highly volatile and therefore almost exclusively passes into the flue-gas stream by the incineration and of the captured mercury nearly 100% ends up in the flue gas cleaning residues. The type of residues depends in the cleaning techniques. Flue gas cleaning residues are typically landfilled but in some EU Member States residues are e.g. mixed with asphalt for road construction (BREF, 2006). In total some 6.8 tonnes mercury per year is disposed of with residues from the incineration. It is here assumed that it all ends up in landfills.

According to the new EU policy, where possible, waste that cannot be recycled or reused should be safely incinerated, with landfill only used as a last resort. This policy is implemented in the new Waste Framework Directive by including energy efficient incineration as a recovery operation (EC, 2008). If it is assumed that all polyurethanes with mercury catalyst in the waste stream ends up in waste incinerators the emission would be more than 3 times higher than the current estimate, corresponding to about 2.3 tonnes/year.

B.9.5.3.2 Landfilling

Based on the distribution described above it is estimated that 25.2 tonnes (18.4 + 6.8) mercury is ultimately landfilled; either as municipal solid waste or as residues from waste incineration.

In the case of landfill fires, mercury in combusted PU is expected to be released 100% to the air. No data have been available for estimating the quantities of waste combusted in landfill fires in the EU.

The guidance for estimation of exposure from waste life stage (ECHA, 2008e) states that various models exist to predict releases from landfills, but none of these models are sufficiently checked against reality to suggest substance specific release factors. The guidance proposes either to assume that landfills are outside the scope of the assessment or to treat substances in landfilled waste as a prolonged service life. Using the latter option the guidance suggests a general annual release factor of 0.05% to air and 3% to waste water (before treatment). However, the guidance document points out that the need for a long-term release assessment should be decided on a case-by-case basis, in particular for metals or organic substances that are persistent and toxic.

During decomposition of the PU in the landfill mercury may be released and e.g. end up in landfill gas, evaporate through the landfill cover or leach with landfill leachate. Investigations that studied Hg emissions from municipal landfills report substantial releases of Hg from municipal landfills. According to Lindberg *et al.* (2005), concentrations in air downwind from municipal landfills were up to 80-fold higher than measured upwind. Hg is released predominantly as elemental mercury (Hg0), dimethylmercury and to some extent methylmercury. According to Mukherjee *et al.* (2004) Hg in waste in the EU has been estimated to 1900 and 4000 t Hg for the year 1995 and consisted of mining waste, waste from

metal and chlorine plants, laboratory waste, residues from incineration, paints, wastes from paper, metal and cement industry and used products like batteries, thermometers, instruments, electronic equipment and light bulbs.

Southworth *et al*. (2005) and Lindberg *et al*. (2005) emphasize that highest Hg-emissions occur at the working face of municipal waste landfills where waste is dumped, distributed and compacted. Lindberg *et al*. (2005) report emission rates ranging from ~1–10 ng $m^{-2}hr^{-1}$ over aged landfill cover, from ~8–20 mg/hr from landfill gas flares (landfill gas flares included Hg^0 at $\mu g/m^3$ concentrations), and from ~200–400 mg/hr at the working face. In the inventory of product related emission in the EU, Kindbom and Munthe (2007) use an emission factor of 0.6%, representing the total atmospheric emission the first 10 years after disposal, for batteries and other product groups (a higher emission factor is applied for measuring and control instruments, light sources and electrical equipment). This is quite well in accordance with the annual emission factor of the guidance document of 0.05% to air which will be used here.

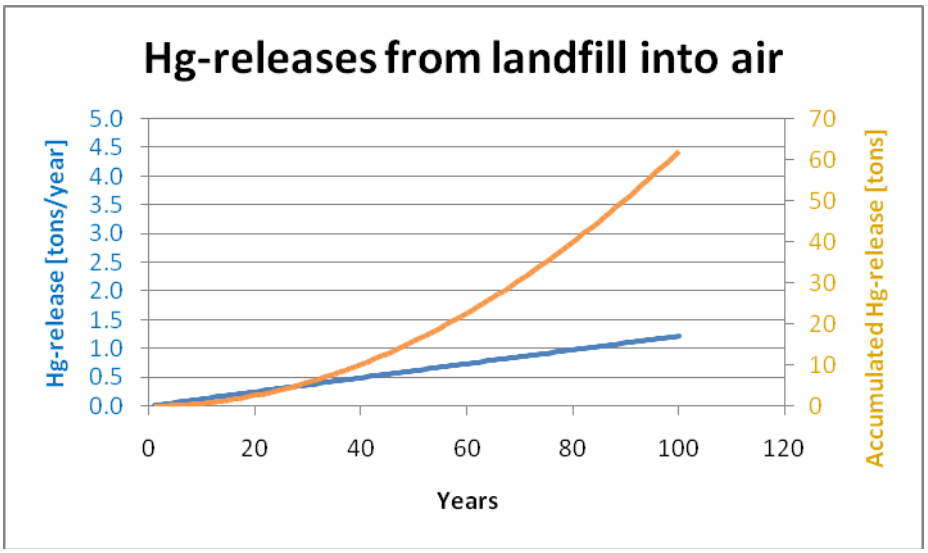
Phenylmercury compounds have to be emitted from polyurethane either as inorganic or as organic mercury before they can be released into landfill gas or leachate water. With a half life of 16 years for Hg in PU (ATSDR, 2008), the release rate of Hg from PU is 4.94E-06 1/h. After 20 years, about 58% of the mercury is likely to be released from polyurethane.
According to the Guidance document on REACH Chapter R.18, the release estimation from landfill needs to consider the residence time of the substance in the landfill body. The substance is continuously applied together with PU-waste to the landfill and accumulates there until its closure. For the derivation of the default RF proposed in the Table R.18- 4 of the TGD, “it is assumed that the average residence time is 20 years. Hence, the annual release factor of the substance during service life is multiplied by the residence time of 20 years to obtain the RFs for the landfill" p. 46.

The default emission factor for air is 0.05% for volatile compounds and corresponds to releases of substances to air during service life (ERC 10a). Releases are estimated based on the OECD emission scenario document on plastic additives (OECD, 2004), which is considered to be inadequate for mercury containing catalysts in polyurethane (see chapter B 9.4.1). Therefore, a default emission factor of 0.05% is considered too low for mercury release from landfills. However, also an emission factor equal to that for service life (9-10%), seems unrealistic and overestimates releases from municipal landfills.

In the inventory of product related emission in the EU, Kindbom and Munthe (2007) use an emission factor of 0.6%, representing the total atmospheric emission the first 10 years after disposal for batteries and other product groups (a higher emission factor is applied for measuring and control instruments, light sources and electrical equipment).

An emission factor of 1% for a residence time of 20 years is therefore considered as a realistic worst case estimate for atmospheric emissions of mercury from landfills. Assuming this emission factor, the release rate of mercury from municipal landfills is 5.7E-08 and thus two orders of magnitude less than the release rate of mercury from polyurethane. Accordingly, Hg release from a landfill is not be limited by the release of Hg from polyurethane waste but by other landfill specific processes affecting the emission of Hg from landfills.

If the emission factor of 1% is applied, the total emission to air from landfilled waste over a 20-years period can be estimated at 0.25 tonnes. This will be used for the tier 1 emission estimate.



Hg –release from landfills at annual application rates of 27 tonnes of Hg with polyurethane waste.

Figure B.9-1 Annual (blue line, left y-axis) and accumulated (orange line, right Y-axis) mercury releases from landfill into air

Using an annual release factor of 3% to waste water would imply that 60% of the mercury is released to waste water over a 20-years period, which is very unlikely. The total releases from municipal landfills in Denmark in 2001 was estimated at 2.5 kg Hg (releases from the amount of mercury accumulated over the years in the landfills) while the amount directed to landfill was 400-2,300 kg (Christensen *et al*., 2004), indicating the releases of mercury the landfill leachate is very small.

According to the estimations a large amount of mercury will accumulate in the landfills and apparently remain there. The long-term fate of mercury in the landfill is not known, evidently there is a potential for a release to the environment at a later stage.

B.9.5.4 Waste water treatment

The total annual mercury releases is estimated at 0.28 tonnes/year.

The major release to waste water treatment is assumed to be from the service life. The fate of the mercury by the waste water treatment will depend on the actual treatment techniques. Danish investigations of balances of mercury by waste water treatment showed that on average 53% of the mercury in the inflow water ends up in the sewage sludge while the remainder was discharged to the recipients. Whether a similar distribution can be expected for the phenylmercury compounds is not known.

The fate of the mercury in the sludge depends on the final disposal of the sludge. ICON (2001) reports that 70-80% of the mercury is transferred to the sewage sludge during conventional urban waste water treatment. They further note that, atmospheric volatilisation

of Hg as methylmercury, formed by biotransformation processes, is a possible mechanism contributing to the removal of this element during secondary wastewater treatment by the activated sludge system, but they note that it is unlikely that this is a major route of Hg loss because of the significant quantities of Hg recovered in the activated sludge.

On an EU level 40% of the overall sludge production is reused (mainly in agriculture) while landfilling and incineration in some Member States is the most widely used disposal method (European Commission, 2009). If it is assumed that 50-80% of the mercury ends up in the sludge, and 40% of the sludge is spread on agricultural soils, it can be roughly estimated that around 0.07 tonnes mercury per year, from the use of mercury catalysts, ends up on agricultural soils.

B.9.5.5 Summary of emissions

The estimated emission factors are summarized in Table B-58 below. The estimated emission of elemental mercury from all life cycle stages is summarized in Table B-59 below.

Table B-58 Release factor used for estimation of emissions

Emission factors				
Life cycle stage	Air	Waste water	Soil	Total
Manufacturing	>0.0025	>0.0006	-	>0.003*
Formulation and prosessing	0.075	0.0006	0.00001	0.076
Service life	0.095	0.010	-	0.105
Waste incineration	0.100	0.0002	-	0.100
Landfilling	0.01	-	-	0.001

* emissions estimate from manufacture data are underestimated, but these underestimations could not be quantified.

Table B-59 Release of mercury and mercury compounds and amounts landfilled from all life cycle stages in tonnes Hg from Phenylmercury Neodecanoate

Life cycle stage	Emissions to air	Emissions to waste water		Amount landfilled
Manufacturing	>0.00192*	>0.00013*		-
Formulation and processing	2.35	0.02		-
Service life	2.75	0.26		18.4
Waste incineration	0.75	~0		6.76
Landfilling	0.25	-		-
Total emission	>6.10*	>0.28*		25.16**
		>6.38*		?**

Assuming a steady state consumption the numbers presented in Table B-59 shows the annual mercury released in tonnes Hg/year. This forms the basis for the risk assessment performed below.
*emissions estimations from manufacture data are underestimated, but these underestimations couldn't be quantified.
**insufficient information is available on long-term fate and behaviour of Phenylmercury compounds and their degradation/transformation products after landfilling.

Emissions in the EU from imported articles and emissions outside the EU from exported articles are not included in these calculations.

The total flow of mercury during the life cycle of mercury catalysts is shown in Figure B9.1. The estimates are based on maximum figures for production and use in articles. For production and export the mercury content has been calculated on the basis of the figures for phenylmercury acetate (60% Hg), phenylmercury 2-ethylhexanoate (48% Hg) and phenylmercury neodecanoate (45% Hg).

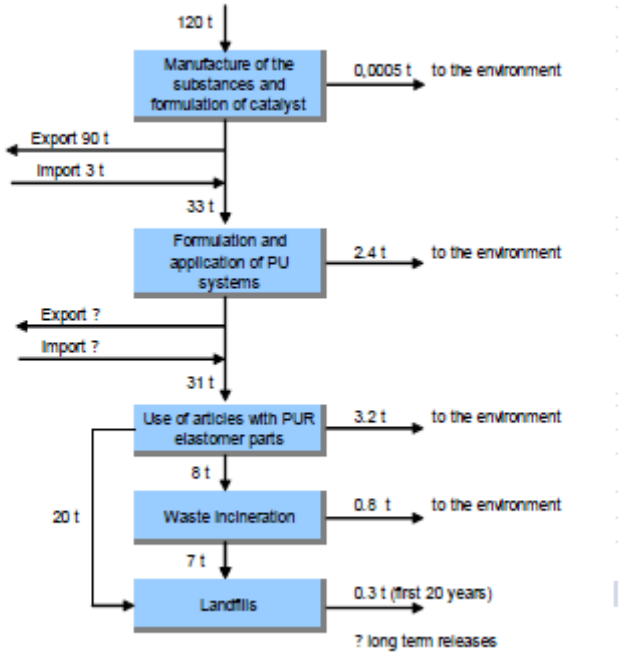


Figure B.9-2 Mercury flow in 2008 (tonnes Hg/year, based on maximum figures for production and consumption) associated with the used of mercury catalysts for polyurethane

The estimated release of 6.1 tonnes Hg/year to air (based on 2008 figures concerning manufacture and use of the substances in EU + EFTA) was compared to the estimated total air emission of mercury from sources in Europe in 2005, that was estimated to be 150 tonnes Hg/year (uncertainty ±30 %) according to UNEP Chemicals Branch[11], 2008 . The total emission from the use of mercury-containing PU is consequently estimated to be in the order of magnitude of 4% compared to the total emissions in Europe in 2005.

New data on emissions of mercury from sources in EU has become available. Mercury emissions to air from anthropogenic sources in EU-27 are reported to be approximately 87 tonnes in 2008[12] (the reported emissions in 2005 to air were 99 tons), while emissions to

[11] Global Atmospheric Mercury Assessment: Sources, Emissions and Transport, December 2008: http://www.unep.org/hazardoussubstances/Mercury/MercuryPublications/GlobalAtmosphericMercuryAssessmentSourcesEm/tabid/3618/language/en-US/Default.aspx

[12] European Union emission inventory report 1990 — 2008 under the UNECE Convention on Long-range Transboundary Air Pollution (LRTAP), Technical report No 7/2010 http://www.eea.europa.eu/publications/european-union-emission-inventory-report

water are reported to be around 5 tonnes in 2008[13]. The estimated release from the manufacturing and use of phenylmercury compounds in catalysts (in EU + EFTA) is 6.1 tonnes Hg/year to air (based on 2008 figures concerning manufacture and use of the substances) consequently the total emissions from the use of phenylmercury catalysts in PU can be estimated to be in the order of magnitude of 7% compared to the reported total emissions to air in 2008 in EU-27 (and in the order of magnitude of 6 % compared to the reported emissions to air in 2005).

It should be noted that the release estimates in the dossier are based on maximum tonnages for production and consumption and the release factors are mainly based on defaults due to lack of more specific information. The estimated releases to air and water may therefore be considered as conservative. However, according to the estimations the major amount of mercury from this source will accumulate in the landfills and apparently remain there. The long-term fate of mercury in the landfill is not known, evidently there is a potential for a release to the environment at a later stage.

Since the use of phenylmercury compounds in PU as a source for mercury emission has not been in focus until recently, the release of mercury from this use is most likely not included in the estimates of total European/EU emissions in the reports mentioned above.

Considering the uncertainties in estimated and reported emissions it can be roughly estimated that the manufacture and use of the substances in EU+EFTA contributes to about 4 to 7 % of the total air emissions of mercury.

Baseline, Estimated future emissions

Table B-60 shows the estimated emissions of Hg from the use of Phenylmercury Neodecanoate in the EU between 2008-2030 representing the baseline. The estimated emissions follows the same downward sloping trend as the estimated future use presented in B.2. The estimates are calculated on the basis of the releasefactors presented in Table B-58 combined with the assumptions given below. The calculations of this baseline also take into account emissions in 2008 from products sold the previous years in contrast to Table B-59 which presents total emissions during the lifecycle of the Phenylmercury Neodecanoate used only during year 2008.

The assumptions for calculating the emissions are as follows:

- It is assumed that use of the substances will decline in line with the estimates provided in the baseline (cf. B.2.3). It is further assumed that environmental releases change in proportion to use.
- It is assumed that releases to air and waste water are the most critical as regards exposure and potential for environmental harm. Releases to landfill are only relevant when subsequently released to other environmental media (except in the context of potential controls on hazardous waste disposal).
- It is assumed that the average product lifetime is 5 years. Whilst it is recognized that several products may have longer lifetimes than this (e.g. flooring is assumed to be 10 years in the exposure assessment), several of the product types detailed earlier in the

[13] The European Pollutant Release and Transfer Register (E-PRTR) http://prtr.ec.europa.eu/PollutantReleases.aspx

assessment are likely to have much shorter timescales and thus 5 years is assumed to be reasonable.

- Emissions from manufacturing are not included in this analysis because they are considered to be negligible based on the above.
- For emissions from formulation and processing, emissions are assumed to occur in the year in which use takes place.
- For service life emissions, emissions in a specific year are assumed to be 1/5 of the releases from those products that enter into use in that year (assuming 5 years product lifetime), plus 1/5 of the releases from products entering into use 4, 3, 2 and 1 years previously.
- Emissions from waste incineration are based on the emissions in 2008 multiplied by the fraction of 2008 usage. It is assumed that products will not enter the waste phase and hence be incinerated for five years (the assumed product lifetime).
- Emissions from landfills in 2008 are, in the exposure assessment, calculated to be 0.25t over a period of 20 years. Therefore, if a steady state were to apply, annual emissions would be 0.25t, relating to products land filled over the previous 20 years. This is based on an emission factor of 0.01 and the amount assumed to be disposed of to landfill (25.2t).
- For the purposes of this analysis, emissions from landfills are assumed to occur with a 5 year lag due to the assumed service life of the products.

Table B-60 Baseline emissions, 2008 and onwards

Baseline emissions, 2008 and onwards		
Year	Downscaling factor	Total emissions
2008	1.00	7.67
2009	0.91	7.05
2010	0.83	6.50
2011	0.76	5.99
2012	0.69	5.52
2013	0.63	5.10
2014	0.58	4.71
2015	0.53	4.36
2016	0.48	4.03
2017	0.44	3.74
2018	0.40	3.47
2019	0.36	3.23
2020	0.33	3.00
2021	0.30	2.80
2022	0.28	2.30
2023	0.25	2.10
2024	0.23	1.91
2025	0.21	1.75
2026	0.19	1.59
2027	0.18	1.45
2028	0.16	1.33
2029	0.15	1.21
2030	0.13	1.10

2031	0.12	1.01
2032	0.11	0.92
2033	0.10	0.84
2034	0.09	0.77
2035	0.08	0.70
2036	0.08	0.64
2037	0.07	0.58
2038	0.06	0.53
2039	0.06	0.48
2040	0.05	0.44

See Appendix 11.

B.9.6 Overall environmental exposure assessment

B.9.6.1 Predicted environmental concentrations

Environmental concentrations at the regional level have been calculated by the EUSES version 2.03 program and using the default regional environmental parameters (TGD, Part II, table 12 p. 88), see Appendix 6. It was not considered feasible to calculate local concentrations based on the information available.

Due to lack of data and also due to the fate of phenylmercury compounds in the environment it is proposed to perform the quantitative risk assessment for environment on the basis of inorganic mercury, The calculations have been performed using the substance properties of phenylmercury acetate (which is the only of the compounds for which sufficient data are available), however assuming that the substance is not biodegradable (as elemental mercury was identified as the relevant component for risk assessment). This worst case release estimation was based on the total consumption volume in the EU + EFTA of all five compounds in terms of elemental mercury, i.e. 31.3 tonnes/year (if mercury/phenylmercury compounds ratio is refined, this value can be rounded to 32 t Hg/year), and the distribution of releases to the environment as summarised in Section B.9.5.5. Calculated PECs regional is presented in Appendix 1.

B.9.6.2 Measured levels

No monitoring data on the phenylmercury compounds themselves in the environment have been found. The phenylmercury compounds are degraded in the environment to give hazardous degradation products, i.e. inorganic mercury and elemental mercury, which can be transformed to methylmercury. Monitoring data on mercury in general are presented in appendix 8.

B.9.6.3 Selected environmental concentrations for risk characterisation

A quantitative risk assessment for the environment is presented in Appendix 1. Due to lack of data, but also due to the fate of the phenylmercury compounds in the environment, it is proposed to perform the quantitative risk assessment for environment on the basis of the inorganic mercury data. However, it should be borne in mind that a piece by piece risk assessment of releases of mercury and mercury compounds from single product groups does

not give the full picture of the risks, for that purpose different sources of releases would have to be combined.

The PBT-assessment shows that degradation/transformation products, i.e. methylmercury, is a PBT like substance. The main objective of the emission characterisation for a PBT/vPvB substance is to estimate the amounts of the substance released to the different environmental compartments during all activities and uses. If transformation/degradation products with PBT-properties are being generated, the substances themselves must be treated like PBT-substances with regard to emission estimation and exposure control. To this end, the exposures and emissions to humans and the environment should be minimized to the extent possible. See also Section B.8.2 Emission characterisation.

B.9.7 Issues related to exposure to exported substances

All the substances are exported as preparations with the phenylmercury compounds dissolved in a solvent and according to manufacturers it is expected that the preparations are solely used as catalysts for formulation of PU systems. Both phenylmercury acetate and phenylmercury 2-ethylhexanoate have been used extensively as biocides in paint and it cannot be ruled out that some of the exported compounds are in fact used as biocides.

The releases from the preparation of the catalysts within the EU are included in the estimated releases from manufacturing the substances.

The processes for formulation of the PU systems and the applications will take place outside the EU and are expected to be more or less the same as for uses within the EU. According to the export notifications in the European Database Export Import of Dangerous Chemicals (EDEXIM) preparations with phenylmercury neodecanoate are to some extent exported to developing countries and the same is probably true for preparations with the other substances. No specific export notifications have been identified for the preparations with phenylmercury acetate and phenylmercury 2-ethylhexanoate. The export of the substances may be covered by the 35 export notifications of "mercury compounds" in 2009.

It must be expected than in general fewer precautions are taken to reduce occupational exposure and releases to the environment for the PU systems when used in developing countries. Further, most developing countries lack systems for management of hazardous waste, and waste from formulation and applications most likely ends up in uncontrolled landfills.

Environmental releases from the handling of waste of mercury-containing articles and waste from the application of the PU systems must be expected to be significantly different for exported catalysts as compared to the uses within the EU. A smaller part of the waste will be incinerated, but for the part incinerated an emission factor well above the emission factor of 10% applied for the EU must be expected. An emission factor of 50%, as applied by Kindbom and Munthe (2007), are more likely for waste incinerators without mercury-specific flue gas control. In a report on global emission from burning mercury-containing products, Maxson (2009) applies for most regions of the world emission factors of 50% and 80% for municipal solid waste incinerators with and without emission controls, respectively, and an emission factor of 60% for open burning of waste and landfill fires.

A significant part of the waste will end up in uncontrolled landfills and dumpsites. In many countries it is common practice to reduce the volumes of the waste by using open fires in the dumpsites and by burning of the mercury-containing polyurethane the mercury compounds will be broken down to elemental mercury and released to the air as elemental mercury or inorganic mercury compounds (e.g. mercury oxide).

As the releases from the manufacturing of the substances and mercury catalyst are very small compared to the release later in the lifecycle, for exported products nearly 100% of the total releases from all lifecycle stages will take place outside the EU. Furthermore, the total lifecycle release of phenylmercury substances used outside the EU may likely be significantly higher than the lifecycle releases of substances used within the EU, mainly due to higher releases from waste disposal operations.

According to information from manufacturers of the substances, the export of phenylmercury acetate and phenylmercury octanoate has been declining and the export is expected to cease by the end of 2010. The reason is a decline in the demand for the substances and increasing costs of manufacturing the mercury compounds within the EU due to significant increases in the prices of pure mercury and increasing cost of complying with environmental requirements. It has not been possible to obtain a clear indication of the trend in the export of phenylmercury neodecanoate. However, the manufactured volume seems only to be slightly declining and the same is probably true for the export.

B.10 Risk characterisation

B.10.1 Human health

B.10.1.1 Workers

Risk from exposure to phenylmercury compound when applying PU systems for casting of PU parts:
In a Tier 1 exposure scenario for an open application of the PU systems for casting of PU parts exposure was estimated by using ECETOC TRA tool with phenylmercury acetate (PMA) data as input. When using activity duration of <15 minutes and 1-4 hours, respectively, the following inhalation exposure estimates were obtained:

- Duration 1-4 hours: 0.084 mg/m^3 (0.05 mg/m^3 Hg)
- Duration < 15 minutes: 0.014 mg/m^3 (0.008 mg/m^3 Hg)

The corresponding DNEL for PMA for 8 hours exposure is 0.00074 mg/m^3. The DNEL is set for PMA. No DNEL is available for phenylmercury neodecanoate.

Assuming that the work involving exposure to PMA would take place in maximum four hours per day and by adjusting the exposure concentration from 4 hours to 8 hours using Haber´s rule and comparing it to the derived DNEL the resulting RCR is 0.084/2 * 1/0.00074 = 57

Using a higher tier tool as the Advanced REACH Tool (ART) to refine the exposure assessment was not possible due to limited information available. Measurments from companies using the PU systems were not available.

A risk is indicated when using a Tier 1 tool, however refining the exposure assessment was not possible due to scarce data.

Risk from exposure to mercury vapour in gymnasiums:
A DNEL for elemental mercury was derived for workers at 1.33 µg/m^3 for long-term, inhalation, systemic effects. The level of mercury vapour in air in gymnasiums with polyurethane floor containing phenylmercury catalysator is reported in Section B.9.3.2.2, and ranges from 0.13 to 2.9 µg/m^3, when non-detectable level reported from one gymnasium is disregarded.

Comparison of the exposure measured by using Lumex Mercury Analyzer to the derived DNEL gives resulting RCR ranging from 0.01 to 2.2.

This indicates a risk for teachers if it is assumed that the staff stays in the gymnasiums 8 hours/day and if the ventilation is turned off.

As described in chapter B.9 the Lumex instrument gives a snapshot of the exposure in a very short time interval, and is strictly speaking not applicable for assessing 8 hours exposure. However Bealieu *et al*. (2008) also applied sampling onto carulite tubes (average ~8 hours) during abatement work followed by analysis using NIOSH Method 6009 for Mercury. The average ~8 hour exposure 0.2µg/m^3 indicates no risk to the abatement workers. Corresponding average measured by using the Lumex instrument was 0.5 µg/m^3.

B.10.1.2 Consumers

Phenylmercury acetate. Quantitative risk characterisation based on estimated air concentration (theoretical) and derived DNEL for PMA

Most probably a large number of different articles may lead to minor exposure of the general population. Wear and tear of surfaces may lead to increased emissions as mercury may be released from the articles and from the part of the surface which is exposed by the abrasion. In some in-door applications high levels of abrasion may be expected, e.g. gymfloorings and rollers on swivel chairs. A theoretical quantitative estimation of possible air concentration of PMA in a bedroom from wheels on a swivel chair has been made, by applying the Guidance R.17. The estimated air concentrations of PMA have been compared with the derived DNEL for PMA, and indicate a risk from consumer products. The quantitative risk characterisation for PMA is presented in Appendix 1.

Mercury Vapour. Risk characterisation based on measurements in school gymnasiums

Polyurethane flexible floor coverings containing PMA as a catalyst were developed in the 1950s and installed in school gymnasiums in the U.S. between the 1960s and the mid 1990s, and probably also in Europe. Mercury released from the floors and recently analyzed by two methods – direct-reading instrument (Lumex) as well as by collection of air followed by analysis (NIOSH method 6009 Mercury) – was found in air as mercury vapour (ATSDR 2008, 2006, 2003; Beaulieu *et al*., 2008). The concentration of mercury vapour in several schools, were more than 10 times higher than the Reference Concentration (RfC) set by the US EPA. These studies indicate that consumer exposure to articles like floorings containing phenylmercury compounds may cause a risk of adverse health effects. For a comparison of the measured values in school gymnasiums with the derived DNEL for elemental mercury, please see Appendix 1, which shows that the majority of measurements from gymnasium floors reported result in a RCR>1, and hence that the risk is not adequately controlled.

This estimation of RCR includes the DNEL derived from the LOAEC regarding exposure to a continuous 24 hours/day, 7 days/week. In reality consumers (as pupils and students) would not be exposed continuously, but for a few hours each week and for a limited numbers of years. However, it should be recognised that the measurements were made in gyms long time after the floorings were new, exposures may be assumed to have been much higher in rooms with new floorings.

B.10.2 Indirect exposure of humans via the environment

As previously mentioned sufficient information is not available to make a quantitative risk assessment of the risk from the exposure of man via the environment from the phenylmercury compounds or their degradation/transformation products. It is, however, evident that the life-cycle of the substances leads to a significant release of mercury to the environment (mainly to air). This was estimated at around 4% of the estimated European emissions of mercury in 2005 and at around 7% of the reported emissions to air for EU-27 in 2008. It has to be noted that mercury and methylmercury may also be generated from other sources than phenylmercury compounds. Once emitted, mercury enters the complex biogeochemical cycle. Mercury is present in fish and seafood products largely as methylmercury. Food sources other than fish and seafood products may contain mercury, but mostly in the form of inorganic

mercury (EFSA, 2004). Risk characterization of man via environment is moved to Appendix 1 (chapter 3.1.2), since it is based on general information on intake of methylmercury from fish and seafood products. In summary the estimated intake of mercury in Europe varies between countries, depending on the amount and the type of fish consumed. The mean intakes were in most cases below the JECFA PTWI[14] of 1.6 µg/kg body weight but high intakes may exceed the JECFA PTWI. Small children seem to be more likely to exceed the PTWI than adults (EFSA, 2004).

B.10.3 Environment

Qualitative risk characterisation based on degradation products with PBT like properties

The PBT-assessment shows that one of the main degradation/transformation products of phenylmercury compounds, methylmercury, is a PBT like substance. According to REACH, if transformation/degradation products with PBT-properties are being generated, the substances themselves must be treated like PBT-substances with regard to emission estimation and exposure control. To this end, the exposures and emissions to humans and the environment should be minimized to the extent possible.

Based on the available information it is estimated that around 75 – 150 tpa of phenylmercury compounds are manufactured for use in the production of phenylmercury catalysts in EU+EFTA, of which 40 – 85 tpa are exported. A substantial amount of phenylmercury compounds are manufactured exclusively for export. The estimated EU + EFTA consumption is approximately 36-70 tonnes (mainly phenylmercury neodecanoate), which corresponds to a total mercury content of approximately 16 – 31.5 tonnes/year, this includes a minor import.

The use of the catalysts is wide dispersive. The total number of companies applying the mercury-containing PU systems is not known but likely several thousands. Moreover, the mercury catalyst is incorporated into the polymer structure and remains in the final product. The mercury-based products are used both for the professional market and for consumer products. The life-cycle of the substances used in the EU+EFTA is estimated to lead to a release of 6.6 tpa of mercury to the environment, mainly to air. This was estimated at around 4% of the estimated European emissions of mercury in 2005 and at around 7% of the reported emissions to air for EU-27 in 2008. Main releases are assumed to be from formulation and processing (large number of sites), service life and the waste phase. Once emitted, mercury enters the complex biogeochemical cycle. The formation of methylmercury under certain environmental conditions and subsequent biomagnification through food webs is of concern.

Quantitative risk characterisation

The PBT-assessment concludes that the phenylmercury compounds themselves are not PBT or vPvB-substances and therefore also a quantitative risk assessment approach can be used. However, due to lack of data and also due to the fate of phenylmercury compounds in the environment it is proposed to perform the quantitative risk assessment for environment on the basis of the inorganic mercury data. The quantitative risk characterization is presented in Appendix 1. It should be borne in mind that a piece by piece risk assessment of releases of mercury and mercury compounds from single product groups does not give the full picture of the risks, for that purpose different sources of releases would have to be combined.

[14] The FAO/ WHO Joint Expert Committee on Food Additives (JECFA) established a provisional Tolerable Weekly Intake (PTWI) for methylmercury to 1.6 µg/kg body weight (WHO, 2003).

B.11 Summary on hazard and risk

Based on the information obtained it is estimated that around 75 – 150 tpa of phenylmercury compounds are manufactured for use in the production of phenylmercury catalysts in EU+EFTA, of which 40 – 85 tpa are exported. 36 – 70 tpa of phenylmercury compounds in catalysts (i.e. 16 – 31.3 tpa calculated as mercury) are used per annum in the EU+EFTA, this includes a minor import. A substantial amount of phenylmercury compounds are manufactured exclusively for export.

The assessment of the five phenylmercury compounds is mainly based on data for phenylmercury acetate since most information is available for this substance. Due to the fact that the phenylmercury compounds are degraded in the environment to give hazardous degradation products, i.e. inorganic mercury and elemental mercury, which can be transformed to methylmercury, the risks that might arise from the degradation/transformation products is considered as well. Based on the information in Section B.4 it is evident that the life-cycle of the substances leads to a significant release of mercury to the environment (mainly to air). This was estimated at around 4% of the estimated European emissions of mercury in 2005 and at around 7% of the reported emissions to air for EU-27 in 2008. Once emitted, mercury enters the complex biogeochemical cycle.

B.11.1 PBT assessment

Phenylmercury compounds

Phenylmercury acetate, phenylmercury propionate, (2-ethylhexanoato)phenylmercury, phenylmercury octanoate and phenylmercury neodecanoate fulfil the REACH Annex XIII toxicity (T) criterion but are not considered to fulfil the persistency (P) criterion or the criterion for bioaccumulation (B) in REACH. The five phenylmercury compounds themselves are therefore not considered as PBT or vPvB substances.

Degradation/transformation products

Fish appears to strongly accumulate methylmercury. Most of the methylmercury in fish tissue is covalently bound to protein sulfhydryl groups. This strong binding is the reason for a long half-life of about two years in biota and as a consequence methylmercury is biomagnified significantly through the food web. With BCF factors in fish in the range of 8140 up to 85700 methylmercury clearly fulfils the REACH Annex XIII criteria for bioaccumulation (B) and the criteria for very bioaccumulative (vB). The criteria for toxicity (T) with a NOEC of 0.26 µg/l for a *Daphnia magna* reproduction test and a provisionally agreed classification of methylmercury as Repr. Cat 1; R61, Repr. Cat 3; R62 and T; R48/25 is also fulfilled. Moreover, methylmercury is highly toxic to birds as described in literature where field observations indicate that in certain fish-eating avian species (divers, sea eagle, fish eagle), intoxications and reproductive impairment were noted after eating fish contaminated with methylmercury at concentrations of 0.2 to 0.7 mg/kg.

Concerning the persistency (P) criteria the facts that demethylation occurs at a much lower rate than methylation under certain environmental conditions and that the biological half-life of methylmercury is high should be judged as of equivalent concern. As documented (B.4) the release and degradation of the phenylmercury compounds contributes to the pool of elemental

and inorganic mercury which cannot be broken down to any harmless form. The cycling of mercury means that the source of methylmercury in the environment is always present once released. The measured environmental concentrations of mercury and methylmercury and the increasing trends of methylmercury levels in biota are of concern Overall, it is concluded that methylmercury is a PBT like substance or a substance of equivalent concern.

B.11.2 Substances forming PBT like substances. Qualitative risk assessment

The PBT-assessment shows that degradation/transformation products, i.e. methylmercury, is a PBT like substance. According to REACH, if transformation/degradation products with PBT-properties are being generated, the substances themselves must be treated like PBT-substances with regard to emission estimation and exposure control. To this end, the exposures and emissions to humans and the environment should be minimized to the extent possible.

The use of the catalysts is wide dispersive. Moreover, the mercury catalysts are incorporated into the polymer structure and remain in the final article. The mercury-based products are used both for the professional market and for consumer products. The life-cycle of the substances used in the EU+EFTA is estimated to lead to a release of 6.4 tpa of mercury to the environment (6.1 tpa to air) in 2008. This was estimated at around 4% of the estimated European emissions of mercury in 2005 and at around 7% of the reported emissions to air for EU-27 in 2008. Main releases are assumed to be from formulation and processing (large number of sites) service life and the waste phase. Once emitted, mercury enters the complex biogeochemical cycle. The potential for formation of methylmercury, that is a PBT like substance, is of major concern and is the main reason for proposing the restrictions.

Sufficient information is not available to make a quantitative risk assessment of the risk from exposure of man via the environment from the phenylmercury compounds or their degradation/transformation products, in particular methylmercury. Mercury and methylmercury may be generated from other sources than phenylmercury compounds, however, it is evident that the life-cycle of the phenylmercury compounds leads to a significant release of mercury to the environment.

General information concerning indirect exposure of man via the environment and the levels of methylmercury in fish and seafood products is given in Appendix 1 (chapter 3.1.2). In summary the estimated intake of mercury in Europe varies between countries, depending on the amount and the type of fish consumed. The mean intakes were in most cases below the JECFA PTWI[15] of 1.6 μg/kg body weight but high intakes may exceed the JECFA PTWI. Small children seem to be more likely to exceed the PTWI than adults (EFSA, 2004).

B.11.3 Quantitative risk assessment.

The PBT-assessment concludes that the phenylmercury compounds themselves are not PBT or vPvB-substances and therefore also a quantitative risk assessment approach can be used. However, due to lack of data and also due to the fate of phenylmercury compounds in the

[15] The FAO/ WHO Joint Expert Committee on Food Additives (JECFA) established a provisional Tolerable Weekly Intake (PTWI) for methylmercury to 1.6 μg/kg body weight (WHO, 2003).

environment it is proposed to perform the quantitative risk assessment for environment on the basis of the inorganic mercury data. However, it should be borne in mind that a piece by piece risk assessment of releases of mercury and mercury compounds from single product groups does not give the full picture of the risks, for that purpose different sources of releases would have to be combined.

Risk was identified for industrial workers exposed to the phenylmercury catalyst during open application of the PU systems for casting of PU parts. Exposure was estimated by using ECETOC TRA tool with phenylmercury acetate (PMA) data as input. Risk was also identified for teachers exposed to mercury vapour from PU floors in gymnasiums, based on measurements with a direct detecting instrument.

The quantitative risk characterisation for consumers indicates that phenylmercury acetate release from articles in the indoor environment is not controlled and may cause adverse health effects to consumers. Measurements of high levels of mercury in air (in the form of metallic mercury) in school gyms with phenylmercury catalyst in floorings clearly show that the compounds are released from articles and degraded. For the use of phenylmercury catalyst in gym floorings the majority of measurements of air concentrations of elemental mercury in school gyms reported would result in a RCR>1, i.e. a risk.

The quantitative risk characterisation for environment indicates that the estimated concentrations of mercury (in the form of inorganic mercury resulting from emissions of the phenylmercury compounds) were below those predicted to cause an effect in the aquatic and terrestrial environment. It should be noted that only a very approximate quantitative risk characterisation for the environment, based on predicted environmental concentrations of inorganic mercury, could be performed. Moreover, due to lack of data a quantitative risk assessment for secondary poisoning could not be performed.

C AVAILABLE INFORMATION ON ALTERNATIVES

C.1 Identification and availability of possible alternative substances and techniques

As identified in Section B.2.2 the main current application of the five phenylmercury chemicals is as catalyst for polyurethane CASE applications (coatings, adhesives, sealant and elastomers).

Alternatives to mercury catalysed PU systems can basically be divided into three groups:

- Same PU systems with non-mercury catalyst (using the same polyol and isocyanate components).
- Other PU systems with non-mercury catalyst (reformulating the system using other polyol or isocyanate components).
- Non-mercury systems based on other polymers e.g. silicones.

Alternative catalysts are marketed today by major suppliers of catalysts for polyurethane elastomers systems. Information on capability of the manufactures indicates that the companies can easily manufacture enough catalyst to replace mercury catalysts under REACH (specific information not provided here due to confidentiality reasons).

Catalysts based on organotin/amine and bismuth/zinc carboxylates have been on the market for years, whereas other alternatives (based on zirconium and titanium), specifically targeting the remaining uses of mercury, have been introduced quite recently, and building up experience in the use of the systems for replacing mercury catalysts is still ongoing. Organotin compounds are not specifically marketed as alternatives for the current uses of mercury catalysts.

According to the trade organisations ISOPA and ALIPA many companies have reformulated their systems because alternatives with the same performance as the mercury catalyst were not available (ISOPA, 2009).

Non-mercury systems based on other polymers may certainly replace mercury containing polyurethane systems for some applications, but a comparison between polyurethanes and other polymers is highly complicated for the wide range of applications of mercury containing polyurethane systems. Non-mercury catalysts seem to be available for almost all applications, and the replacement is mainly a question of some research and development for finding the right catalyst and application technique.

C.1.1 Mercury catalysts

C.1.1.1 Properties of mercury catalysts

In polyurethane manufacture, for many applications, the catalysts of choice for catalysing the reaction between a polyol and an isocyanate composition, i.e., for hardening or curing polyurethane (PU) materials, have long been organic mercury compounds. This is because, for a wide range of polyurethane materials, these catalysts provide a robust and desirable "reaction profile" with the following characteristics:

- They discriminately catalyse the reaction of isocyanate and polyol rather than the competing disadvantageous side reaction of isocyanate and water.
- They provide urethane forming reaction mixtures of relatively long gelation time (pot life) and relatively slow buildup of viscosity. A reasonable induction time before hardening is desirable because it allows the liquid reaction mixture to be cast or spread after addition of the catalyst, and therefore gives the user more control over the application. A rapid and complete reaction after the gel time is important to provide finished articles that are not sticky and that develop their desired physical properties.
- That they are inert to moisture.

For certain applications these catalysts should have special properties like long induction time (also known as the “gel time” or “pot life), with a sharp viscosity rise toward the end of the reaction, followed by a “fast” curing of the part. In contrast to PU foam manufacture, the formation of bubbles and foam is undesirable in polyurethane CASE applications. For this reason, mercury and other heavy metals have long been used as catalysts as they exhibit the high reactivity and selectivity required in the process.

Nowadays, mercury catalysts only account for a minor part of the market for PU CASE catalysts, but when considering alternatives it is essential to address the catalysts that actually have similar properties as mercury catalysts. It is common to use terms like "mercury-free" in the description of PU catalysts and PU CASE systems, but this does not necessarily indicate that the catalysts can be considered as alternatives to mercury catalysts. In the recent years, when environmental concern with respect to the use of mercury catalysts has emerged, "mercury-free" is also used for catalysts in areas where mercury catalysts have not been used for many years, if ever.

C.1.1.2 Catalysts mentioned in the patent literature

Mercury catalysts are organo-mercury salts containing an aromatic or aliphatic radical that is bonded directly to divalent mercury and is inert to isocyanate polyol reactions. The catalysts have a high solubility in the urethane-forming reaction mass and in the polyol reaction component.

The general formula of organo-mercury catalysts which may be used as alternatives is

$(R\text{-}Hg)_n\text{-}X$

wherein R is aryl, aralkyl, alkaryl, heterocyclic or straight, branched alkyl, or cyclic lower alkyl, and the halo, amido, carboxy, lower alkoxy or nitro substituted derivatives thereof. Different descriptions of patents dealing with organo-mercury catalysts for polyurethane production, mention the following aryl groups: benzyl, phenyl, napthyl, anthryl, phenanthryl. Typical alkaryl groups comprise α-tolyl or aralkyl such as phenylethyl or phenyloctyl groups. Heterocyclic groups comprise furfuryl or imidazolyl groups

X is an anion and comprises typically a saturated or unsaturated mono- or dicarboxylate with between 2 and 18 atoms. Also halogenated derivates of these carboxylates can be used. The following carboxylates are mentioned in different descriptions of patents that deal with

organo-mercury catalysts for polyurethane production: acetate, propionate, benzoate, methacrylate, hydroxide, phthalate, salicylate, octoate, stearate, butyrate, valerate, heptanoate, octanoate, 2-methylhexanoate, hexanoate, nonanoate, decanoate, dodecanoate, octadecanoate, dodecenyl succinate, octenyl succinate, gluconate, decenyl glutarate, octyladipate and octodecyl malonate, p-chlorophenylmercury aacetate and p-chlorobenzoate.

n is an integer of 2-4 and the mercury is bound directly to the carbon atoms of the nucleus R.

Possible catalysts are mentioned in several patent descriptions. Here, we refer to the catalysts mentioned in the United States Patent 3419509, 3429855, 3642044, 4256848 that gives a representative but not complete list of organomercury catalysts:

2,4-bis[(formato)mercuri]benzene and the 1,2- and 1,4-bis isomers thereof
2,4-bis[(acetato)mercuri]benzene and the 1,2- and 1,4-bis isomers thereof
2,4-bis [(acetato)mercuri]-3-chlorobenzene
2,4-bis[(propionato)mercuri]benzene and the 1,2- and 1,4-bis isomers thereof
2,4-bis[(acetato)mercuri]-5-nitrobenzene
1,4-bis[(benzoato)mercuri]benzene and the 1,2- and 1,3-bis isomers thereof
2,4-bis[(benzoato)mercuri]-5-bromobenzene
1 ,4-bis[(benzoato)mercuri]-5-nitrobenzene
2,4-bis[(isobutyrato)mercurij-bromobenzene and the 1,2- and 1 ,4-bis isomers thereof
1 ,4-bis[(octoato)mercuri]benzene and the 1,2- and 1,3-bis isomers thereof
2 ,4-bis[(sterato)mercuri]5 ,6-dichlorobenzene
1,2,3-tris[(propionato)mercuri]benzene
1,3,4,6-tetrakis [(propionato)mercuril]benzene
1,2,3-tris[(benzoato)mercuri]benezene
2,4-bis[(propionato)mercuri]naphthalene
1,2,5,6-tetrakis[(naphthenato)mercuri]naphthalene
1 ,4,5,8-tetrakis[(propionato)mercuri]anthracene
1,6-bis[(benzoato)mercuri]phenanthrene
2,4-bis[(propionato)mercuri]-5-amido benzene
2,4-bis[(benzoato)mercuri]-5-methoxy benzene
a,a-bis[(benzoato)mercuri]toluene
a,a-bis[(propionato)mercuri]toluene
a,a-bis[(benzoato)mercuri]-ethyl toluene
a ,a-bis[(propionato)mercuri]-4-chloro toluene
a,a-bis[(benzoato)mercuri]-4-carboxy toluene
di-(mercuri benzoato)ethane
1,3-(dimercuri benzoato)propane
1,4-(dimercuri benzoato)cyclohexane
1,4-(dimercuri propionato)-5-chlorocyclohexane
3,4-(dimercuri benzoato)nonane
1,18-(dimercuri propionato)octadecane
2,4-bis[(propionato mercuri)]furan

2,3,5-tris[(benzoato mercuri)] imidazole
2,4-bis[(propionato mercuri)]5-nitroimidazole
2,4-bis[(benzoato mercuri)]oxazole

phenylmercury acetate
o, m, or p-chlorophenylmercury acetate
o, m, or p-bromophenylmercury acetate
phenylmercury propionate
phenylmercury 2-ethylhexanoate
o, m, or p-fluorophenylmercury acetate
chloromethyl mercury chloracetate
methyl mercury decanoate
phenylmercury phenoxide
methyl mercury benzonate
phenylmercury oleate
phenylmercury nitrate
2-acetoxymercuripyridine
phenyl mercuric octanoate
p-tolyl mercury acetate
phenylmercury butyrate
p-methoxyphenylmercury acetate
phenylmercury p-cholorobenzoate
phenylmercury neodecanoate
phenylmercury dodecanoate
phenylmercury 2,2 dimethyl hexanoate
phenylmercury decenoate
tolylmercury octanoate
tolylmercury dodecanoate
bis(chlorophenylmercury) octyl adipate
tertiary butylmercury decanoate
phenylmercury 2,2-dimethylhexanoate
bis(phenylmercury) dodecenyl succinate
bis(phenylmercury) decenyl succinate
bis(tolyl mercury) dodecenyl succinate
bis-(tertiary butylmercury) dodecenyl succinate

C.1.1.3 Marketed alternative mercury catalysts

Currently, at least two additional mercury compounds are possibly marketed for use as a catalyst in PU systems.

The substance [μ -[(oxydiethylene phthalato)2-)]] diphenylmercury (CAS No 94070-93-6) is used in the catalyst Cocure 44 from Vertellus (Vertellus 2006). The molecular structure of the compound is shown below:

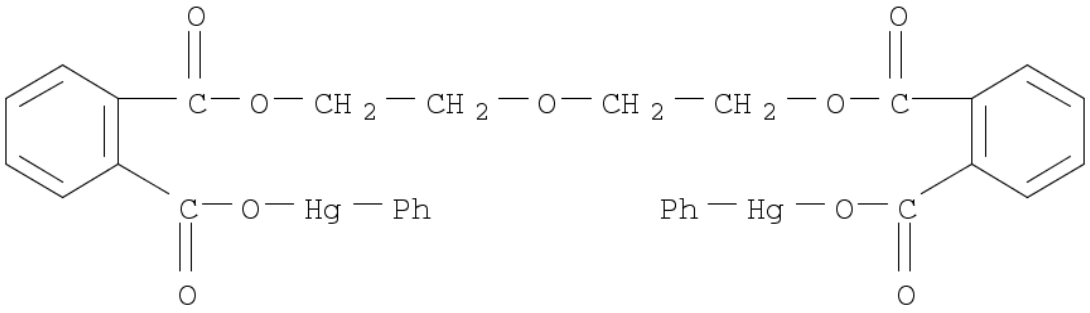


Figure C.1-1 Molecular structure of [μ -[(oxydiethylene phthalato)2-)]] diphenylmercury (marketed as Cocure 44)

According to information from suppliers, the catalyst is used for systems where clarity is important. Mentioned applications are PU systems for skateboard wheels and coatings. Other examples of the use of the substance are two systems manufactured in the USA: Huntsman RP 6405 polyurethane hardener with 0.1-0.2 % of the substance and Brunswick Curethane CU-100 Topcoat Resin.

According to the European Database Export Import of Dangerous Chemicals (EDEXIM), a substance indicated as bis(phenylmercury)tetradecylsuccinate was exported from Spain to South Africa and Brasil in 2010. The export of the substance may indicate that it is manufactured within the EU.

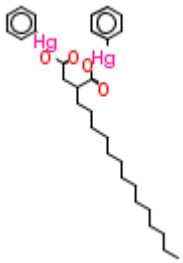


Figure C.1-2 Molecular structure of bis(phenylmercury)tetradecylsuccinate

It has not been possible to identify the CAS number of the substance and the list of pre-registered substances does not include a compound with this name.

The substance is very similar to the substance bis(phenylmercury) dodecenylsuccinate (CAS No. 27236-65-3) (molecular structure shown in Figure C.3) that is pre-registered to ECHA under the name diphenyl[μ-[(tetrapropenyl)succinato(2-)-O:O']]dimercury. . Besides the use as catalysts the substance is in the literature reported to be used as a biocide and fungicide.

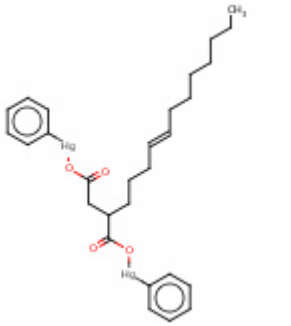


Figure C.1-3 Molecular structure of bis(phenylmercury) dodecenylsuccinate

A MSDS for a polyurethane elastomer systems from BCC PRODUCTS, INC. (USA) indicates that this substance (CAS No. 27236-65-3) is used as a curing agent. The substance is also listed in MSDSs from other companies including Vishay Measurements Group Inc, Hastings Plastics and BJB Enterprices, Inc (all from the USA). The mercury content is indicated at <0.04 to 0.06 %. It has not been possible to find European suppliers for this substance.

Several other MSDSs only indicate that the product contain a "proprietary aryl mercury compound" at a concentration of 0.083%.

A Taiwanese chemical manufacturer of fine chemicals market a solvent-free catalyst, TAC 535, which consists of a "phenylmercury ester of a C10 monocarboxylic acid" (Repoly, 2005). The exact chemical name and the CAS No are not informed. The substance may likely be phenylmercury neodecanoate which is an ester of a C10 monocarboxylic acid and the indicated mercury content of 35% is similar to the content indicated for one of the marketed catalysts with phenylmercury neodecanoate.

C.1.1.4 Previously marketed catalysts

A patent from 1980 on a coating system for application of a moisture proof barrier to a substrate makes reference to an aryl organo-mercury catalyst marketed under the trade name Cocure 23 (Patent 4,195,009, 1980). Cocure 23 is, however, not marketed today, and no information on this aryl organo-mercury compound is available.

C.1.1.5 Inorganic mercury compounds

No references to the use of inorganic mercury compounds as catalyst in PU systems have been identified. It is deemed to be very unlikely that manufacturers would shift to the use of inorganic mercury compounds instead of shifting to mercury-free substances, because it in any case would imply some process changes and research and development.

C.1.1.6 Pre-registered substances

A large range of organo-mercury carboxylates and polycarboxylates are pre-registered at ECHA's web-site. At least 20 of the pre-registered substances (including 4 of the 5 substances covered by this Annex XV dossier) would fall within this group, and may in principle be used as catalyst in PU systems (see Table C-1 below). In addition, a few other substances may fall within the group, but the evaluation would require a closer assessment of the structural formula of the substances than has been done within this assessment. Apart from Cas No 27236-65-3, which is used as catalyst today, no data have been available to evaluate the efficiency of the different compounds and to what extent the compounds would have a reaction profile similar to the profile of the mercury catalysts applied today. A search on the Internet using the CAS No and MSDS only gave positive results for PU systems for Cas No 27236-65-3.

Table C-1 Alternative mercury catalysts within the group of organo-mercury carboxylates and polycarboxylates that are pre-registered

Cas Number	Chemical name (as pre-registered)
94-43-9	phenylmercury benzoate
104-59-6	phenylmercury stearate
108-07-6	(acetato-O)methylmercury
109-62-6	(acetato-O)ethylmercury
122-64-5	Lactatophenylmercury
124-08-3	2-ethoxyethylmercury acetate
151-38-2	2-methoxyethylmercury acetate
584-18-9	2-hydroxy-5-(1,1,3,3-tetramethylbutyl)phenylmercury acetate
2701-61-3	(maleoyldioxy)bis[phenylmercury]
3626-13-9	methylmercury benzoate
22450-90-4	amminephenylmercury(1+) acetate
23319-66-6	[2,2',2''-nitrilotri(ethanol)-N,O,O',O'']phenylmercury lactate
27236-65-3 *	diphenyl[μ-[(tetrapropenyl)succinato(2-)-O:O']]dimercury
27605-30-7	[2-ethylhexyl hydrogen maleato-O']phenylmercury
31632-68-5	[naphthoato(1-)-O]phenylmercury
61792-06-1	[(2-hydroxyethyl)amino]phenylmercury acetate
93882-20-3	[μ-[[4,4'-(oxydiethylene) bis(dodecenylsuccinato)](2-)]]diphenyldimercury
94070-93-6	[μ -[(oxydiethylene phthalato)2-)]] diphenylmercury

* Used as catalyst in marketed PU curing agents.

C.1.1.7 Summary, mercury catalysts

Many different organic mercury compounds can be used as catalysts in polyurethane production (see Section C.1.1.2). COWI and Concorde (2008) reported that: "Well over 100 mercury chemicals are marketed in the EU (e.g. Chemos, 2008). 41 of these compounds were selected for further investigation, and actual sale on the EU market has been confirmed by the

industry for more than 75% of the selected compounds. In addition, there are significant imports and exports of mercury compounds between EU and non-EU countries."

During consultations for the work with the Cowi and Concorde 2008 report a list of mercury chemicals was compiled based on lists from different suppliers. A questionnaire was sent to the major suppliers and they were asked to indicate the use of the substances and to indicate the total EU volume. Only some of the suppliers responded and the information obtained was further scrutinized in an interview with some of the suppliers. The aim of the study was to get an impression of which substances were the most important and their volumes, this on a very approximate level. The survey did not focus on minor uses or uses as intermediate in chemical or pharmaceutical industry. Moreover, chemicals that are contained in imported articles were not possible to identify at all (e.g. the diphenylmercury compound described in Section C.1.1.2). A large consumption of certain phenylmercury compounds, included in this restriction proposal, was identified.

In the consultations for the Annex XV restriction report (two consultations), industry was asked specifically about the substances previously identified which are now included in the restriction proposal (initially 4 based on the former report but a fifth substance was identified).

No information was received on other functions of these 5 substances besides as catalyst, biocide and pesticide. We can assume they are (only) used for the function as catalyst in EU today as they are not allowed in biocides or plant protection products (a possible exception of use in cosmetics as preservative but that use was not indicated by industry during consultations). The substances are also manufactured in large volumes for export.

Regarding the whole group of possible mercury alternatives, and in particular the "organo-mercury carboxylates and polycarboxylates" that are pre-registered, we cannot exclude that they may be used as catalysts, but it may be assumed that this use is not very extensive. Moreover, it cannot be excluded that there may be other uses, e.g. as intermediates in chemical or pharmaceutical industry. In this area the information gathered for this report may not be complete. The fact that 20 of the possible alternative organo-mercury compounds are pre-registered may indicate that they are manufactured in or imported to EU for some use.

C.1.2 Catalysts marketed as mercury catalyst alternatives

In the following, a number of catalysts, specifically indicated by the manufacturers of the catalysts as alternatives to mercury catalysts, are described.

A large number of mercury-free catalysts for PU elastomers have been developed as alternatives to mercury – the large number reflecting the fact that there does not appear to be a single "drop-in" substitute for mercury catalysts that can be used in all the different systems, that confers similarly desirable curing properties, and that is as easy to adjust to the needs of the user.

According to a major supplier of catalysts, the consumption of mercury catalysts is today probably only 1/3 of the consumption ten years ago, reflecting the fact that alternatives have been applied for a number of applications. The alternatives applied so far seems mainly to be organotin compounds, bismuth/zinc carboxylates and tertiary amines. The remaining mercury applications are mainly those applications for which the replacement of the mercury is not

straight forward. Organotin compounds are not specifically marketed as alternatives for the current uses of mercury catalysts.

C.1.2.1 Catalysts based on bismuth and zinc carboxylates

According to Shepherd Chemical Company "Bismuth-based carboxylates have remained the "state-of-the-art" choice for replacement of mercury or lead-based catalyst in polyurethane elastomers and coatings" (Si-Ahmed, without date). In the early 1980's the company developed the BiCAT® line of polyurethane catalysts which according to the manufacturer enabled formulators and manufacturers to replace the prevailing mercury, lead and tin catalysts with a viable alternative.

The BiCAT® series consist of 14 products with different organobismuth and organozinc compounds. A number of the products consist of bismuth neodecanoate or bismuth tris(2-ethylhexanoate) (also designated bismuth octoate) in different mixtures with organic acids. Two representative examples, one also with zinc neodecanoate, are shown in the following table.

Table C-2 Examples of the composition of catalysts in the Bicat series recommended as alternatives to mercury containing catalysts. (Source: MSDS from Shepherd Chemical Company)

BiCat	Chemicals	CAS No.
BiCat 8	Bismuth neodecanoate	34364-26-6
	Zinc neodecanoate	27253-29-8
	Neodecanoic acid	26896-20-8
BiCat HM	Bismuth 2-ethylhexanoate (bismuth octoate)	67874-71-9
	2-Ethylhexanoic acid	149-57-5

According to Si-Ahmed (paper without date), despite commercial successes, the bismuth compounds require formulators to adjust for the different reactivity of bismuth in comparison to mercury. The most apparent difference between bismuth-based and mercury-based compounds is the viscosity increase as the urethane reaction proceeds. In addition, some formulas catalyzed with bismuth alone show a tackiness in the finished polymer, especially under high humidity conditions. As a solution to this the company developed a catalyst based on a mixture of bismuth neodecanoate and zinc neodecanoate (BiCat 8). Using the dual metal catalyst the formulator has the ability to adjust the gel behaviour by changing the concentrations of the two metals in the system. Generally, bismuth supplies all the gelling speed necessary to cure an elastomer, while zinc, being a much slower gel catalyst, and better a cross-linking catalyst, accelerates the "back-end" of the reaction (Si-Ahmed, without date).

Organobismuth and organozinc are also used in the series of alternative catalysts by Vertellus Specialties Inc., which also market the mercury-based Cocure® catalysts. According to the manufacturer "*The Coscat® products are proprietary organobismuth and organozinc compounds specifically developed as catalysts for 2-component polyurethane systems. These products were designed to impart performance similar to that of the organomercurial compounds, which are highly selective toward the isocyanate-hydroxyl reaction as opposed to the isocyanate-water reaction, thus avoiding bubble generation at low levels of moisture*." (Vertellus, 2010). The series consists of five catalysts Coscat® 28, Coscat® 83, Coscat® 8330, Coscat® BiZn and Coscat® Z-22. Examples of the compounds are bismuth

neodecanoate and zinc(bis(2-ethylhexonate), but for some of the products proprietary bismuth and zinc compounds are used.

Some of the compounds are recommended for use in combination. According to the manufacturer, Coscat® 83 catalyst (with proprietary organobismuth catalyst) "provides a reduced toxicity alternative to organo-metallic carboxylates based on lead, mercury or tin without sacrificing performance" (Vertellus, 2009c). According to the producer, Coscat® 83 catalyst can produce fast gelling systems, however, in soft to medium hardness systems the final stage of cure can lag resulting in surface tack. The addition of Coscat® Z-22 (with proprietary organozinc compound) can reduce this lag in final cure, yielding a stronger final cure typical of a mercurial catalyst. Vertellus has been requested information on applications where the Coscat® catalysts cannot replace the mercury-based Cocure® catalysts, but no answers have been obtained.

C.1.2.2 Catalysts based on zirconium carboxylates

King Industries Speciality Chemicals produce the K-KAT® XK-604 based on zirconium carboxylates. According to the MSDS "K-KAT XK-604 is an effective catalyst for the reaction of isocyanates and polyols with hydroxyl groups used in the production of cast elastomers. It is a proprietary mixed organometallic complex specially formulated to be an alternative to mercury catalysts without the toxicity concerns." (King Industries, 2007). According to the manufacturer, K-KAT XK-604 can potentially be used in all of the 2-component urethane elastomer applications including castable elastomer (i.e., wheels or rollers), reaction injection moulded parts (i.e. body panels, window encapsulation), adhesive (i.e., construction, automotive and textile) and sealant applications. K-KAT XK-604 was developed to provide an alternative to mercury catalysts mainly based on the reaction profile. According to the manufacturer they have found that, in many cases, the reaction profile of K-KAT XK-604 catalyzed, 2-component polyol/isocyanate reactions are similar to systems catalyzed with mercury, particularly when the isocyanate is aromatic, for example MDI (methyl diphenyl diisocyanate). In many cases the company also found that, compared to commercial mercury catalysts, lower levels of K-KAT XK-604 could be used. K-KAT XK-604 can be added directly to the polyol component of a two-component system. King Industries Speciality Chemicals also produce a number of other catalysts for PU systems including catalysts with bismuth carboxylates (e.g. K-KAT 348 for elastomers) and aluminium chelate (K-KAT 4205 for two-component urethane coatings).

One of the drawbacks of the bismuth and zirconium system seems to be their sensitivity to moisture. According to King Industries a common catalyst problem is the hydrolysis of bismuth and zirconium systems in the presence of water (King Industries, 2000). The solution is for the zirconium catalysts to add the catalyst to the isocyanate component, whereas for the bismuth catalyst it is to add a moisture scavenger (King Industries, 2000). Both, however, may be inconvenient for the user of the PU system.

C.1.2.3 Catalysts based on titanium chelates

Johnson Matthey Plc. has developed the SNAPCURE™ 2000 series. According to the manufacturer, "The SNAPCURE™ 2000 series has been designed to replace mercury catalysts in MDI elastomer applications" (Johnson Matthey, 2009). The SNAPCURE™ series can be used in polyester, PTMEG (polytetramethylene ether glycol) and most polyether

polyols, provided the latter are >80% primary alcohol. The products are fully compatible with a variety of fillers and chain extenders and can be pre-mixed with the polyol. The SNAPCURE™ profile is similar to mercury in the way that they provide a variety of pot-lives, good hardness build-up and improved de-mould and tack free times. Further, according to the manufacturer, they give minimal promotion of the isocyanate-water reaction.

The series consists of five products with different properties: SNAPCURE 2120, 2130, 2200, 2210, 2220. They are all based on titanium chelates. Chelation is the bi- or multidentate binding or complexation of a single metal ion by chelating agents (also called ligands). These chelating agents, which are often organic compounds, form a chelate complex with the metal ion inactivating the ions so that they cannot normally react with other elements or ions. The titanium chelates are mixed with different organic compounds e.g. diethylene glycol or isopropanol in order to obtain the desired reaction profile.

C.1.2.4 Catalysts based on organotin compounds

One part of the mercury catalyst replaced so far has been replaced with organotin catalysts. These organotin compounds have been used for replacing some applications of mercury but are not specifically marketed as alternatives for the current uses of mercury catalysts.

As an example the Cotin® Organotin Catalysts series from Vertellus, recommended for silicone and polyurethane systems, included catalysts based on dibutyltin diacetate (CAS No 1067-33-0), dibutyltin dilaurate (77-58-7), dimetylbis[(1-oxoneodecyl)oxy]stannate (CAS No 68928-76-7), dibutyltin oxide (818-08-6) and dioctyltin dilaurate (3648-18-8). The catalysts are used for different PU systems, e.g. major end uses for the catalyst based on dibutyltin dilaurate include rigid and flexible polyurethane foams, coatings, adhesives, sealants, elastomers and casting compounds (Vertellus 2009d).

According to a brochure from Reaxis Inc. (U.S.A) "The trend toward replacing mercury catalysts in polyurethane elastomers propelled us to develop ReaxisTM C317 and employ co-catalysis to achieve similar reaction profiles (Reaxis, 2009)". According to the brochure from the company's web site, ReaxisTM C317 contains dibutyltin bis-(isooctyl maleate). However, the ReaxisTM C317 is not included in the list of products on the company's website, and probably not manufactured anymore.

The risks of organotin compounds in general are high. Due to severe health and environmental effects, several restrictions have been imposed regarding organotin compounds in the EU. Organotin compounds are not included in the Review Programme under the Biocidal Products Directive 98/8/EC and organotin containing biocides are no longer lawfully on the European market. According to REACH Annex XVII the following provisions apply; Organostannic compounds are restricted for use as biocide in paints and in antifouling systems on ships. Furthermore tri-substituted organostannic compounds (TBT, TFT) are prohibited in articles (in concentration greater than the equivalent of 0.1% by weight of tin). From 2012 dibutyltin (DBT) compounds are prohibited in mixtures and articles for supply to consumers (general public), by derogation the provisions apply from 2015 for certain specified applications, e.g. in certain types of sealants and adhesives and in paints and coatings when applied on articles. Dioctyltin (DOT) compounds are prohibited from 2012 in certain specific consumer articles. These restrictions should be considered as a clear signal that organostannic compounds are not suitable alternatives.

C.1.2.5 Catalysts based on amines

In order to find mercury-free, non-toxic catalysts for CASE applications with a long pot life and sharp viscosity rise the Japanese Tosoh Corporation examined the effectiveness of various metal and tertiary amine catalysts (Kometani *et al*., year not indicated). The authors concluded that a catalyst system based on tertiary amines produced the desired properties: a long pot life, sharp viscosity rise and excellent elastomer properties. The Toyocat DB series from Toyoh, based in tertiary amine, is marketed as catalyst for polyurethane adhesive, sealant and elastomer applications.

For Toyocat DB-41 the applications area is specifically indicated as: "For Adhesive, Sealant, Elastomer applications as replacement of Sn, Hg. Provides long pot life. Exhibits sharp viscosity build-up profile." (Tosoh, 2009). Toyocat-DB-41 is a special acid blocked catalyst of 50% 1.8-diazabicyclo[5.4.0]undec-7-ene (DBU) in diethylene glycol (Kometani *et al*., year not indicated). According to the authors, DBU alone does not provide a long pot life and TOSOH Corporation has investigated the use of several kinds of blocking agents. Blocking agents can be phenol or organic acids by which the DBA is used in a complexed state. Contrary to mercury catalysts, amine catalysts easily cause foaming problems that increase when the water content of the system is high and Kometani *et al*. (year not indicated) conclude that the water content should be controlled when applying Toyocat DB-41. They further conclude that at small thickness, heat becomes more critical.

In Europe, the Toyocat series are among others marketed by Brenntag UK and Ireland, who specifically indicates the DB series as "Series for CASE applications to replace mercury catalysts" (Brenntag, 2009).

C.1.2.6 Summary

Representative alternative catalyst and information on ingredients listed in the Material Safety Data Sheets are shown in Table C-3 below. In all of the products the organometal or amine catalyst make up a significant part, but percentages of the substances in the product have been excluded for confidentiality reasons.

The main catalysts marketed as alternatives to current uses of mercury catalysts are based on zirconium, bismuth and zinc carboxylates, titanium chelates and tertiary amines.

Table C-3 Selected catalysts for polyurethane CASE applications indicated as alternatives to mercury catalysts by the manufacturers

Product name	Manufacturer	Ingredients according to the MSDS	CAS No
K-KAT® XK-604	King Industries Speciality Chemicals	Zirconium carboxylates	Confidential
BiCat 8	Shepherd Chemical Company	Bismuth neodecanoate	34364-26-6
		Zinc neodecanoate	27253-29-8
		Neodecanoic acid	26896-20-8

BiCat HM	Shepherd Chemical Company	Bismuth 2-ethylhexanoate (bismuth octoate)	67874-71-9
		2-Ethylhexanoic acid	149-57-5
Snapcure™ 2530	Johnson Matthey Catalysts	1,3,5-triazine-1,3,5(2h,4h,6h)-tripropanamine, n,n,n',n',n'',n''-hexamethyl-	15875-13-5
		Titanium(IV) chelate	Not allocated
		Isopropanol	67-63-0
Snapcure™ 2200	Johnson Matthey Catalysts	Diethylene glycol	111-46-6
		Titanium(IV) chelate	Not allocated
		Isopropanol	67-63-0
		Pentane-2,4-dione	123-54-6
Coscat® 83	Vertellus Specialties Inc.	Bismuth neodecanoate	34364-26-6
		Neodecanoic acid	26896-20-8
Coscat® 8330	Vertellus Specialties Inc.	Bismuth neodecanoate	34364-26-6
		Neodecanoic acid	26896-20-8
		Zinc(bis(2-ethylhexonate)	136-53-8
		[methylene)bis(oxy)]dipropanol	24800-44-0
Toyocat DB-41	Tosoh Corporation	1.8-diazabicyclo[5.4.0]undec-7-ene	6674-22-2
		Diethylene glycol	111-46-6
Reaxis™ C317 (may not be manufactured anymore)	Reaxis Inc	Dibutyltin bis-(isooctyl maleate)	25168-21-2

For the assessment of health and environmental risks related to the alternatives in Section C.2 and C.3, data search for the following six specific substances has been conducted:
- Bismuth neodecanoate (CAS No. 34364-26-6)
- Bismuth tris(2-ethylhexanoate) (CAS No. 67874-71-9)
- Zinc neodecanoate (CAS No. 27253-29-8)
- Zirconium carboxylates (CAS No. confidential)
- Titanium(IV) chelate (CAS No. not allocated)
- 1.8-diazabicyclo(5.4.0)undec-7-ene (CAS No. 6674-22-2)

The four substances with CAS numbers have been pre-registered at ECHA with a foreseen registration deadline of 1 December 2010. However, no registration was performed in 2010.

Some general considerations regarding the health and environmental properties of the alternative organometal/metalloid substances are included in Section C.2 and C.3.

C.2 Human health risks related to alternatives

C.2.1 Health properties of the non-mercury substances

The information obtained on the health effects of the specific substances is very sparse as indicated below.

C.2.1.1 Bismuth neodecanoate

No data available for specific health effects assessment.

C.2.1.2 Bismuth tris(2-ethylhexanoate)

According to a safety data sheet from the manufacturer of the substance it is not irritant to skin but causes eye irritation. It is not considered sensitising. No other data on toxicological properties were found.

C.2.1.3 Zinc neodecanoate

According to a safety data sheet from the manufacturer, the substance may cause irritation to skin and eyes, but it is not considered sensitising. No other data on toxicological properties were found.

C.2.1.4 Zirconium carboxylate

No data available for specific health effects assessment.

C.2.1.5 Titanium(IV) chelate

No data available for specific health effects assessment.

C.2.1.6 1.8-diazabicyclo(5.4.0)undec-7-ene

The following data on this amine is presented in a safety data sheet (Alfa Aesar GmbH & Co.KG) for the substance:

LD_{50}, oral rat: 215 - 681 mg/kg
LD_{50}, dermal, rabbit: 1233 mg/kg
Local effects: Corrosive to skin, eyes and mucous membranes. Risk of perforation of oesophagus when swallowing the substance.
Sensitisation: No known sensitising effect
Other effects: Not known
Classification, health: R34 (Causes burns); R21/22 (Harmful by inhalation and in contact with skin)

A mutagenicity study in mouse lymphoma cells has been conducted with and without metabolic activation with negative result. No other information on genotoxicity has been found (CCRIS).

Based on the above, it can be concluded that this possible alternative is less acutely toxic compared to e.g. phenylmercury acetate, it has the same corrosive properties but with regard to other effects, little information is available for comparison.

C.2.2 General considerations regarding the non-mercury organometal/metalloid substances

With regard to the five organo-metal/metalloid substances and different compounds of these substances some general considerations can be made.

C.2.2.1 Bismuth and compounds

Bismuth compounds are considered to be poorly to moderately absorbed following inhalation or ingestion. Absorbed bismuth is distributed throughout the soft tissues and bone, the highest concentrations being found in the kidneys and liver. Absorbed bismuth is excreted primarily via the urine. The biological half-life for whole-body retention is about 5 days but intranuclear inclusions containing bismuth seem to remain for years in the kidney of patients treated with bismuth compounds. High-level exposure causes renal failure with degeneration and necrosis of the epithelium of the renal proximal tubules, fatty changes and necrosis of the liver, reversible dysfunction of the nervous system, skin eruptions and pigmentation of the gums and intestine. For the general population the total daily intake via food is about 5-20 μg, with much smaller amounts contributed by air and water. An important source of exposure for specific segments of the population in the past was the therapeutic use of bismuth compounds. The cosmetic use of bismuth compounds still continues to be fairly widespread (HSDB).

C.2.2.2 Zinc and compounds

Zinc is an essential mineral that is naturally present in some foods, added to others, and available as a dietary supplement. Zinc is also found in many over-the-counter drugs. The average daily intake (AVDI) of zinc for adult humans in the western world is 7-15 mg; mostly from food (HSDB).

Zinc toxicity can occur in both acute and chronic forms. Acute adverse effects of high zinc intake include nausea, vomiting, loss of appetite, abdominal cramps, diarrhoea, and headaches. One case report cited severe nausea and vomiting within 30 minutes of ingesting 4 g of zinc gluconate (570 mg elemental zinc). Intakes of 150–450 mg of zinc per day have been associated with such chronic effects as low copper status, altered iron function, reduced immune function, and reduced levels of high-density lipoproteins. Reductions in a copper-containing enzyme, a marker of copper status, have been reported with even moderately high zinc intakes of approximately 60 mg/day for up to 10 weeks (NIH, 2009). Inhalation of ultra-fine particulate zinc oxide (diameter < 0.1 μm) generated from welding of galvanised steel may cause metal fume fever. Symptoms include dry and sore throat, fever, coughing, dyspnoea, muscular pains, headache, gastro-intestinal disturbance and metallic taste (EC, 2004).

The EU risk assessment reports on different zinc compounds conclude that there are insufficient grounds to classify zinc as genotoxic although results vary widely and conflicting

results have been found even within the same test systems. It is also concluded that there is no indication of carcinogenic action of zinc.

C.2.2.3 Zirconium and compounds

Zirconium and zirconium compounds are of generally low toxicity, although granulomas have been produced by repeated topical applications to human skin e.g. after the application of deodorants containing sodium zirconium lactate or of cream containing zirconium oxide. Zirconium workers have also developed pulmonary granulomas after exposure to zirconium. In rats the oral LD_{50} of several zirconium compounds ranged from 2.5 to 10 g/kg. A study of 22 workers exposed to fumes from a zirconium reduction process for 1 to 5 years revealed no abnormalities referable to the exposure. There are no well-documented cases of toxic effects from industrial exposure (OSHA, 2009).

Although metabolism studies are lacking, it is assumed that significant amounts of zirconium may be absorbed orally from intake of various foods. Lamb, pork, eggs, dairy products, grain, and vegetables contain the highest concentrations, varying generally between 3 and 10 ppm. The daily oral intake in man has been estimated at 3.5 mg. Although its excretory routes have not been adequately studied, the presence of relatively high concentrations of zirconium in the liver and gallbladder suggests that it is probably excreted by the biliary system in the feces, while zirconium levels in the urine are negligible. However, soluble citrate complexes retained in the kidneys are evidently excreted in the urine. Milk is a second route of excretion and significant amounts of zirconium are found in foetuses. Zirconium is neither an essential element nor a toxic element in the conventional sense. The average body burden is 250 mg. The biochemical properties of zirconium include a high affinity for phosphate groups and an inhibitory effect on many enzymes, such as ATPase, pyrophosphatase and blood phosphatases (HSDB, 2009).

The US EPA has included the zirconium salt of 2-ethylhexanoic acid (CAS 22464-99-9) in their HPV Chemical Challenge Programme (US EPA, 2005), i.e. a possible representative of "zirconium carboxylates". The following findings are presented in the document:

One characteristic of hexanoic acid, 2-ethyl, zirconium salt and other metal carboxylates is that they readily dissociate from an ion pair into free metal and free acid. They are found as partially dissociated products in the ambient environment (i.e., neutral pH). Dissociation is a reversible process and the proportion of dissociated salt is dependent on the pH and pKa (the dissociation constant), which is the pH at which 50% dissociation occurs. In the low pH environment of the digestive tract (e.g., pH 1.2) complete dissociation will occur for these metal carboxylates. The transport and bioavailability of the metals and acids are determined by their solubility in environmental media and biological fluids which is determined by environmental parameters such as pH. Results from a study following OECD Guideline 112 indicate that about 50% dissociation will occur at approximately neutral pH (i.e., representative of aquatic and marine ecosystems), while complete dissociation will occur at the physiologically relevant pH of the mammalian stomach (pH 1.2).

Because the free acid (2-ethylhexanoic acid) and corresponding free metal (zirconium) have different characteristics (e.g., solubility, adsorption, and toxicity) than the undissociated salt (ion pair), the proportion of dissociation influences the behaviour of the substance in the

environment and in vivo. The bioavailable fraction of the constituents of metal carboxylate salts can be estimated from the dissociation constants. At the low pH of the mammalian stomach (pH 1,2) all of the metal carboxylates are expected to be completely, or nearly completely, dissociated. This indicates that when administered orally, the absorption and resulting toxicity would be due to the independent action of the carboxylic acid and the free (ionized) zirconium.

Available data from toxicity studies involving 2-ethylhexanoic acid, zirconium 2-ethylhexanoate and zirconium tetrachloride as an example of a salt are presented in Table C-4

Table C-4 Human health endpoints for zirconium 2-ethylhexanoate, 2-ethylhexanoic acid and zirconium tetrachloride (Source: US EPA, 2005)

Human health endpoint	Zirconium 2-ethylhexanoate	2-ethylhexanoic acid	Zirconium tetrachloride
Acute Oral LD_{50}	> 5000 mg/kg (rat)	1600 - 3200 mg/kg (rat)	438 mg/kg (mouse); 700 mg/kg (rat). For $ZrOC1_2$, 1227 mg/kg (mouse); 3500 mg/kg (rat)
Inhalation LC_{50}	> 8.8 mg/L (rat; 1 hr exposure)	> 2.36 mg/L (rat; hr exposure)	Effects observed from inhalation of 6 mg Zr/m3 for 60 days
Dermal LD_{50}	> 5000 mg/kg (rabbit)	< 5.0 m/kg (guinea pig)	-
Skin irritation	Not a primary skin irritant to rabbits; primary skin irritant; guinea pigs	Slight necrosis in rabbits after 4 hrs.	No sensitisation in guinea pigs or mice
Eye irritation	Not a primary eye irritant in rabbit	Severe corneal irritation in rabbits after 24 hours	Zirconium compounds are eye irritants
Repeated dose	-	For 13-week dietary exposure, NOAEL -300 mg/kg-day for rats and -200 mg/kg day for mice	230 mg Zr/kg (as $ZrOCl_2$) did not affect survival, behaviour or growth of rats dosed via gastric tube for 16 days; no effect of 5 ppm $ZrS0_4$ in rats via drinking water over lifetime
Genetic toxicity (in vitro)	Negative in Ames assay with *Salmonella*; negative in bacterial DNA amage/repair assay with *E. coli*	Negative in Ames assay with *Salmonella*	Negative in His' reverse fluctuation assay with *Salmonella*; negative in SOS Chromotest with E. coli.
Genetic toxicity (in vivo)	Negative in mouse micronucleus test	Negative in mouse micronucleus test	Chromosomal abnormalities in mouse bone marrow and human leucocytes($ZrOCl_2$)
Developmental	-	No evidence of teratogenicity. In rats, NOEL = 100 mg/kg/day for offspring, 250 mg/kgday for maternal animals. For rabbits, NOEL = 250 mg/kg for offspring, 25 mg/kg for maternal animals[16]	-
Reproductive	-	NOEL = 300 mg/kg for parental generation, 100 mg/kg for F1 generation (rats)	-

[16] It should be noted that 2-ethylhexanoic acid, CAS no. 149-57-5, is classified as Repr. 2 H361d in CLP Annex VI.

From these results it appears that the zirconium carboxylate has a low acute toxicity, and it was not a primary eye or skin irritant in rabbits but a primary skin irritant in guinea pigs. No repeated dose toxicity studies or reproductive toxicity studies are available for the zirconium carboxylate. The substance was negative in both in vitro and in vivo genotoxicity studies.

From the US EPA HPV Programme it is also reported that zirconium sulphate administered at 5 ppm in drinking water in lifetime studies with rats (where the diet contained an additional 2.6 ppm) indicated no evidence of any biological or toxicological activity of zirconium, except to inconsistently affect the body weight of older animals. There was no evidence that zirconium was tumorigenic in a rat strain (Long-Evans) with appreciable (20%) tumor incidence.

Based on data from the US EPA HPV programme, 2-ethylhexanoic acid showed moderate acute toxicity by the oral route. In a 13 weeks repeated dose toxicity study in rats changes in haematological parameters and organ weights were observed. The effects were however reversible within 28 days. 2-ethylhexanoic acid was negative in Ames test with and without metabolic activation and also negative in the in vivo mouse micronucleus assay. The substance may cause reproductive toxicity and is classified as Repr. 2 H361d in the CLP Annex VI (REGULATION (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures).

With regard to the carboxylic acids in general, these compounds are often exhibiting irritant properties. Other possible adverse effects, like reproductive effects, may depend on carbon-chain length. Information on possible reproductive effects associated with carboxylic acids need further investigation as well as long term effects in general for the carboxylic acids.

C.2.2.4 Titanium

Titanium compounds are generally considered to be poorly absorbed upon ingestion and inhalation. However, detectable amounts of titanium can be found in the blood, brain and parenchymatous organs of individuals in the general population; the highest concentrations are found in the hilar lymph nodes and the lung. Titanium is excreted with urine.

According to available data on the toxicity of titanium and titanium compounds and their presence in various environmental media, there is indication that exposure to titanium does not constitute any health risks for the general population. Studies on titanium alloys, used in implants, do not indicate any adverse local effects on tissues, suggesting that titanium is a biologically compatible element (IPCS, 1982).

C.2.3 Summary

In summary, the health risks associated with the metals/metalloids used in the alternative catalysts are expected to be significantly lower than those of mercury, based on a general assessment of substance reviews and limited specific data. Zirconium and titanium are of low toxicity whereas some adverse effects are seen in relation to excessive intake of bismuth and zinc.

No information is available about the nature of the chelate moiety of the titanium-based alternative and related health effects.

Little information is available on the tertiary amine evaluated, however the acute toxicity is lower than for phenylmercury acetate.

C.3 Environment risks related to alternatives

C.3.1 Environmental properties of the non-mercury substances

The information obtained on the environmental properties of the six specific substances is very sparse, and only in the case of 1.8-diazabicyclo(5.4.0)undec-7-ene has it been possible to establish a limited set of base-data.

C.3.1.1 Bismuth neodecanoate

No data available for specific environmental assessment.

C.3.1.2 Bismuth tris(2-ethylhexanoate)

No data available for specific environmental assessment.

C.3.1.3 Zinc neodecanoate

No data available for specific environmental assessment.

C.3.1.4 Zirconium carboxylates

From the US EPA HPV Chemical Challenge Programme (US EPA, 2005) the following environmental information on zirconium salt of 2-ethylhexanoic acid (CAS 22464-99-9) as a possible representative of "zirconium carboxylates" is presented:

Zirconium 2-ethylhexanoate
Reliable toxicity data not available.
The substance is almost insoluble in water (0.5 μg/l) and has a LogKow of 4.37.

2-ethylhexanoic acid
LC_{50} (96 h), fathead minnow (*Pimephales promelas*) = 70 mg/l
EC_{50} (48 h), daphnia (*Daphnia magna*) = 85.4 mg/l
EC_{50} (96 h), algae (*Scenedesmus subspicatus*) = 40.6-44.4 mg/l
The solubility in water is 25 mg/l and the log Kow is 3.0.

Zirconium tetrachloride (considered to represent Zirconium, Zr)
LC_{50} (96 h), rainbow trout (*Onchorhynchus mykiss*) >20 mg Zr/l
EC_{50} (48 h), daphnia (*Daphnia magna*): reliable data not available
EC_{50} (96 h), algae (*Scenedesmus subspicatus*) = 2.6 mg Zr/l
The substance is soluble in water.

Zirconium oxychloride (considered to represent Zirconium, Zr)
LC_{50} (96 h), bluegill, fathead minnow 15-270 mg Zr/l.

Table C-5 Environmental properties of zirconium 2-ethylhexanoate, 2-ethylhexanoic acid and Zirconium tetrachloride (Source: US EPA, 2005)

Environmental property	Zirconium 2-ethylhexanoate	2-ethylhexanoic acid	Zirconium tetrachloride
Water solubility (mg/L)	0.0005	25	Soluble
LogKow	4.37	3.0	NR
LC_{50} (96 h), fish (mg/L)	No reliable data	70	>20 15-270*
EC_{50} (48 h), daphnia (mg/L)	No reliable data	85.4	No reliable data
EC_{50} (96 h), algae (mg/L)	No reliable data	40.6-44.4	2.6

* Zirconium oxychloride, ZrOCl2.

These data indicate that the aquatic toxicity of the organic moiety of the zirconium carboxylate molecule is low. The toxicity of the zirconium ion to fish is also moderate-low whereas a somewhat higher (although not very high) short-term toxicity to algae of this element is noted. The LogKow of 4.37 of Zr-ethylhexanoate indicates a moderate bioaccumulation potential but no further information on this aspect has been found.

C.3.1.5 Titanium(IV) chelate

No data available for specific environmental assessment.

C.3.1.6 1.8-diazabicyclo(5.4.0)undec-7-ene

This substance has a moderately low vapour pressure of 2 Pa, a high solubility in water at ambient temperature (4920 mg/) and a Log Kow of 1.38 (ChemID). It is not biodegradable in standard laboratory tests (BOD = 0%; TOC = 1 %) and the calculated BCF is <3.6 (Japanese MITI/CERI Database).

According to the database of the supplier (Sigma-Aldrich), the aquatic toxicity of this substance is low:

LC50 (96 h), golden orfe (Leuciscus idus) = 50-100 mg/l
EC50 (48 h), daphnia (Daphnia magna) >50 mg/l
EC50 (72 h), algae >100 mg/l.

The Japanese MITI/CERI database reports an LC50 = 376 mg/l for rice fish (Medaka), Oryzias latipes.

Based on the above, it is concluded that this possible alternative is significantly less toxic in the environment than the phenylmercury compounds, it is not bioaccumulative but appears to be persistent in the environment.

C.3.2 General considerations regarding the non-mercury organometal/metalloid substances

Overall, the metals/metalloids bismuth, titanium, zinc and zirconium are considered to have moderate-low toxicity in the environment (Emsley, 2000). They are not on the list (or on the candidate list) of priority substances in the environmental quality standards Directive (2008/105/EC) under the EU Water Framework Directive (2000/60/EC), and likewise they do not appear on the list of US EPA's water Quality Criteria (2006). This is a good indication of the much lower environmental concern associated with these elements compared to mercury for which strict quality standards/criteria have been set on both the mentioned lists.

Organostannics.

PBT assessment of 4 groups of organostannics

In the RAR, an assessment of the PBT (persistence, bioaccumulation and toxicity) and vPvB (very persistent and very bioaccumulating) characteristics of organotins has been undertaken.

For Persistence, it is likely that the four (groups of) organotins being considered (tributyltin, TBT; dibutyltin, DBT; dioctyltin, DOT and triphenyltin, TPT) will meet the P and vP criteria.

For Bioaccumulation, TPT has a BCF of more than 5,000 (in freshwater species) and, as such, is likely to exceed the B and vB criteria for the marine environment. TBT has a BCF value of more than 3,000 and would thus meet the B criterion but not the vB criterion. However, it is important to stress that this is a value obtained for freshwater species. With regard to marine species, much higher BCF values are reported with particular reference to an inverse relationship with concentration (in other words, the lower the concentration the higher the BCF value). Values of 10,000 and upwards have thus been reported. For DBT and DOT, the BCF values are significantly below 2,000. Given the differences in effects in freshwater and marine environments, it is possible that the corresponding BCF values in the marine environment might be somewhat higher but no reliable data were identified.

For toxicity, TBT and TPT would be classified as T. Furthermore, it is likely that DBT would also be classified as T. However, the situation with DOT is less clear. The freshwater NOEC is above the threshold value and there are insufficient data to demonstrate the use of much lower values in the marine environment.

Table C-6 Potential PBT/vPvB Classification of 4 organostannic groups: dibutyltin (DBT), tributyltin (TBT), dioctyltin (DOT) and triphenyltin (TPT).

Criterion	DBT	TBT	DOT	TPT
P	yes	yes	yes	yes
B	possibly	yes	possibly	yes
T	probably*	yes	possibly	yes
PBT	possibly	yes	possibly	yes
vP	yes	yes	yes	yes
vB	unlikely	yes	unlikely	yes
vPvB	unlikely	yes	unlikely	yes

* SCHER (2006) notes that the classification for DBT as T should be definitely ‘yes’ as opposed to ‘probably’. A careful assessment is, however, required for the B classification.

Overall, it is concluded (with SCHER agreeing) that, in relation to the marine environment, TBT and TPT are likely to be classified as both PBT and vPvB substances. Although DBT and DOT could be classified as PBT substances, they are unlikely to be vPvB substances. It is, however, understood that DOTC is on the European Chemicals Bureau's list for candidate PBT/vPvB substances, subject to further B tests.

Carcinogenic, Mutagenic and Reprotoxic (CMR) of 4 groups of organostannics

According to the ECB website, the final proposal of the Technical Committee for Classification and Labelling of substances for the 30th Amendment to Technical Progress (ATP) of Directive 67/548/EEC includes a proposal for dibutyltin chloride to be classified as a Category 2 reproductive toxin and Category 3 mutagenic substance19. As a category 2 reprotoxic substance, the sale to consumers of preparations containing DBTC will be banned at levels above the limit concentration for exposure as set out in Annex I of Directive 67/548/EEC, relating to the classification, packaging and labelling of dangerous substances. It is worth noting that a similar classification has been agreed by the Commission Working Group on Classification and Labelling for dibutyltin oxide (DBTO); however, this is not listed in the 30th ATP. It is also understood that there is a German proposal (similar to an earlier Swedish proposal) to extend the ECB classification decision for DBTC to a group entry in Annex I for salts of DBT in due course (Rohm & Haas, 2005).

However, in relation to human health risks, it is important to bear in mind that the 'safe' level of exposure for the four groups of organotins (DBT, TBT, DOT and TPT) being considered in this study is determined by other types of effects. Specifically, the opinion of SCHER is that the human health effects for these four groups of organotins are additive both for the target organ (thymus) and for the mode of action (immunotoxicity).

C.3.3 Environmental properties of alternative mercury catalysts

It seems that all organo mercury catalysts have ionic properties and consist of a carboxylate or dicarboxylate anion and an organo mercury cation. In aqueous solutions it can be expected that the substances dissociate into the anion and cation. Differences in dissociation behavior are expected to be marginal as long as the vicinity of the carboxylic group consists of an aliphatic, saturated carbon chain. This means that in waters and soils, degradation of organo mercury catalysts is mainly determined by the organo mercury cation and insignificantly affected by the carboxylic or dicarboxylic group. If the organo mercury cation is phenylmercury, the environmental fate in soil and water is the same as for the 5 proposed phenylmercury compounds. This is probably the case for the marketed substance bis(phenylmercury)tetradecylsuccinate and the pre-registered substances phenylmercury stearate (CAS No. 104-59-6), lactatophenyl mercury (CAS No. 122-64-5), bis(phenylmercury)dodecencylsuccinate (CAS No. 27236-65-3) and other phenylmercury carboxylates such as phenylmercury oleate. However, if the mercury is directly connected to another aromatic, cyclic or aliphatic group, further degradation of the organo mercury cation might be considerably different. Probably, also these substances are finally degraded to inorganic mercury compounds, but degradation times might vary.

In order to assess atmospheric lifetimes for potential organo mercury catalysts, the whole molecular structure of the substances has to be taken into account. The quantum chemical calculations performed by Tang & Nielsen (2010) indicate that atmospheric lifetimes of the 5

proposed phenylmercury carboxylates do not vary considerably. All these compounds consist of an aliphatic, saturated carbon chain. These results indicate that also other phenylmercury carboxylates with aliphatic, saturated carbon chains have similar atmospheric lifetimes of 1 day. Organo mercury substances that contain unsaturated or aromatic carbon structures or are substituted with other atoms probably behave differently and the results of the quantum chemical calculations cannot be extrapolated for these compounds.

C.3.4 Summary

In summary, the environmental risks associated with the metals/metalloids used in the alternatives to mercurycatalysts are expected to be significantly lower than those of mercury, although this assessment is based on very limited specific data. The carboxylic acid moiety of the bismuth-, zinc- and zirconium-based substances is considered to have low toxicity to aquatic organisms. No information is available about the nature of the chelate moiety of the titanium-based alternative.

C.4 Comparison of the risk related properties of the phenylmercury compounds and the alternatives

According to the information given in Section C.1 a large number of mercury-free catalysts for PU elastomers have been developed as alternatives to mercury, and are easily available for most applications.

The main catalysts marketed as alternatives to current uses of mercury catalysts are based on zirconium, bismuth and zinc carboxylates, titanium chelates and tertiary amines. Six specific substances representing all these categories were chosen for the evaluation of the health and environmental properties for the alternatives in Section C.2 and C.3. Some general considerations of the five organometal/metalloid substances and different compounds of these are also included. Limited information is available on the properties of the alternative substances and no REACH registration data is provided so far. In Table C-7a summary of the risk related properties of the phenylmercury compounds used in PU catalysts and the alternative groups of substances are presented.

Other mercury catalysts than the five phenylmercury substances have been used in the past. Some diphenylmercury catalysts are still marketed, and current use in EU can not be excluded. Information on classification of the substances (organic mercury compound entry) is also included in Table C-7.

Table C-7 Available information on the health and environmental related properties of phenylmercury compounds and alternative substances

Substance	Persistence	Bioaccumulation	Toxicity		Classification
			Health	Environ-ment	
Phenylmercury acetate	Low for PhHg, High for MeHg	Low for PhHg, High for MeHg	High	High	Acute Tox. 3 (oral) H301;; Skin Corr. 1B H314; STOT RE 1 H372; Aq. Acute 1 H400; Aq. Chro. 1 H410.
Phenylmercury propionate, 2-ehylhexanoate, octanoate, neodecanoate					Acute Tox. 1 (dermal) H330; Acute Tox. 2 (oral) H310; Acute Tox. 2 (inhal.) H300; STOT RE 2 H373:; Aq. Acute 1 H400; ; Aq. Chro. 1 H410.
Diphenylmercury compounds	Not assessed	Not assessed	High	High	Acute Tox. 1 (dermal) H330; Acute Tox. 2 (oral) H310; Acute Tox. 2 (inhal.) H300; STOT RE 2 H373; : Aq. Acute 1 H400; Aq. Chro. 1 H410.
Bismuth carboxylates	Regarded as lower than MeHg, no information found	Regarded as lower than MeHg, no information found	Lower than PhHg	Low	No harmonised classification for Bismuth neodecanoate (CAS No. 34364-26-6) or Bismuth tris(2-ethylhexanoate) (CAS No. 67874-71-9)
Zinc carboxylates	Regarded as lower than MeHg,	Regarded as lower than MeHg,	Lower than PhHg	Moderate	No harmonised classification for Zinc neodecanoate (CAS

	no information found	no information found			No. 27253-29-8)
Zirconium carboxylates	Regarded as lower than MeHg, no information found	Moderate	Generally low*	Moderate-low	No harmonised classification for Zirconium carboxylates (CAS No. confidential)
Titanium chelates	Regarded as lower than MeHg, no information found	Regarded as lower than MeHg, no information found	Low	Regarded as low	No harmonised classification for Titanium(IV) chelate (CAS No. not allocated)
Tertiary amines	High	Low	Lower than PhHg	Lower than PhHg	No harmonised classification for 1.8-diazabicyclo(5.4.0)undec-7-ene (CAS No. 6674-22-2)
Dibutyltin, Di-octyltin compounds	High	Moderate - possibly high	High	High	Dibutyltin dichloride; Muta. 2; H341 Repr. 1B; H360FD Acute Tox. 2; H330 Acute Tox. 3; H301 Acute Tox. 4; H312 STOT RE 1; H372 Skin Corr. 1B; H314 Aquatic Acute 1; H400 Aquatic Chronic 1; H410

* 2-ethylhexanoic acid, diccociation product of zirconium salt of 2-ethylhexanoic acid may cause reproductive toxicity (classified as Repr 2 H361d)

It's to note that catalysts based on organotin compounds are no longer specifically marketed as alternatives for the current uses of phenylmercury catalysts and were not included in the evaluations of the health and environmental risks of alternatives in Section C.2 and C.3. However, the risks of organotin compounds in general are high (see Table C-7) and the use of several organotin compounds are regulated in the EU, c.f. Section C.1.2.4.

When restricting the use of the five phenylmercury catalysts in polyurethane, there is a risk for substitution with other mercury based catalysts. Such mercury substances are classified according to the entry "organic compounds of mercury" in REACH Annex XVII, cf. Table C-7, Table B.3 and Appendix 7. No specific information has been collected concerning risk related properties for the substances. However, it can be expected that these compounds will also eventually degrade to Hg in the environment. Industry should therefore in all cases seek mercury free alternatives. Restrictions on other mercury containing catalysts could be further elaborated.

Based on the data available, as summarised in Table C-7, the properties of the non-mercury substances marketed as alternatives for the current uses of phenylmercury catalysts are generally regarded as safer than the mercury catalysts with regard to degradation in the environment, potential for bioaccumulation and toxicity. However, entry 20 of Annex XVII of REACH already contains restrictions on organostannic compounds used as biocide in free association paint or to prevent the fouling, or used in the treatment of industrial waters. In addition, Commission Regulation (EU) No 276/2010 completes this annex XVII with a ban on tri-substituted organostannic compounds, and restrictions on dibutyltin compounds and

dioctyltin compounds. These restrictions should be considered as a clear signal that organostannic compounds are not suitable alternatives

C.5 Technical and economical feasibility of alternatives (mercury free)

The consultation undertaken for the socioeconomic assessment (Part F), as well as that undertaken in Section B.2 for the analysis of uses and releases of the substances, indicates that there are significant ongoing efforts and pressures to further replace mercury-based catalysts in polyurethane products. For many of the applications mercury-free alternatives already exist. As a result of this the use of mercury-based catalysts in polyurethane products has already decreased substantially.

Whilst there is significant uncertainty in the rate of future decline, continued decline in use is expected. However, it seems clear that there are some uses of these compounds that will require additional time and effort if their replacement is to be achieved. Therefore, it is unlikely that these substances will be fully replaced by alternatives without any additional regulatory pressure.

In order to understand exactly which uses and products would be most difficult to replace it would be necessary to consult with the actual users of the polyurethane systems. Unfortunately, this has not been possible as the producers of these systems were not willing to give information about their customers due to commercial confidentiality.

C.5.1 Applications for which substitution is particularly difficult

According to a major manufacturer of catalysts, experience shows that the replacement of mercury catalysts has been particularly difficult for the following PU systems (representing about 30% of the total use of mercury catalysts):

- PU elastomer systems with the polyol being a secondary alcohol based polyether. These are usually based on poly(propylene) glycol (PPG) and are typically used for cheaper resin systems with lower quality and product properties. The system is often used for softer elastomers (such as shoe soles and sports tracks). Organotin/amine catalysts have been used for these systems, but according to one industry contact, with varying success. The systems may be replaced with more expensive PU systems with non-mercury catalysts.
- PU elastomer systems with toluene diisocyanate (TDI). TDI based systems are used for niche products within the CASE area (coatings, adhesives, sealants and elastomers).
- PU elastomer systems with aliphatic isocyanates (some success with replacement). Products based on aliphatic isocyanates are used in high performance applications where, for example, extremely high resistance to weathering, high solvent resistance, durable elasticity and protection against aggressive environmental influence are needed (ALIPA, 2009a). Examples are high-quality engineering materials used e.g. for rollers and belts.

Information available from the consultations performed for this study suggests that the uses that could not be substituted within 2 years are for higher performance products for the repair of rubber components or linings for which there is heavy abrasion in use and/or for use in

extreme environments (for example such as in the repair of elastomers in offshore applications in the oil and gas extraction industry). For some of the applications the problem is the humidity sensitivity of the catalysts. They may work if the catalyst is added at the point of use, but this may in some cases not be possible due to equipment limitations. The temperature also plays a role; in some systems alternatives works better in hot cure systems than in cold. The main barriers to the substitution for these types of uses are technical and are associated with finding alternatives that can match the degree of cure and cure speed performance as well as the strength of the final product (for some uses consultation indicated that non-mercury containing substitutes resulted in products with 70% of the required strength, resulting in products not being fit for purpose).

C.5.2 Economic feasibility of alternatives

According to COWI and Concorde East/West (2008) Hg-free PU systems are not in general more costly than mercury-containing PU elastomer systems. In some cases they are even less costly. Therefore, the mere fact of being obliged to use a mercury-free system instead of a mercury-catalysed system does in general not imply any change in cost. The cost of most mercury-free catalysts is quite competitive with the typical mercury catalyst cost. According to COWI and Concorde East/West (2008), quoting industry contacts, the cost of the mercury catalysts have increased significantly in recent years, and was in 2008 in the range of €40-50/kg, compared to €25-35/kg for medium-priced mercury-free catalysts, and €10-20/kg for cheap mercury-free catalysts. A bismuth catalyst would be fairly close to the cost of the mercury catalysts while a tin catalyst (no longer specifically marketed as alternatives for the current uses of the mercury catalysts) would be significantly less expensive.

Information provided by industry contacts for this study indicates that about 70% may be replaced relatively easy while the other 30% are not impossible, but would require additional time. Nevertheless, assuming a clear incentive such as legislation and with the further legislative assurance of a level playing field, within 5 years after a restriction is adopted, virtually all mercury containing polyurethane elastomer systems could be substituted.

C.5.3 Technical feasibility of alternatives

If the Hg-free system has slightly different properties from those of the mercury-catalysed system, then there could be issues of product reliability, etc., at least in the near term, until such problems are worked out (COWI and Concorde East/West, 2008).For some systems the solution may be to shift to more costly PU systems (e.g. by replacing secondary PPG systems). It has not been possible to investigate the extra costs of such adaptions due to the problems mentioned above. It is understood from one producer of polyurethane systems that changes to end products from the use of systems without mercury catalysts would not, in their opinion, result in compromises to the safety of the use of the end products. However, this cannot be ruled out for other companies and uses.

Dow Hyperlast, one of the two dominating companies on the UK polyurethane market, has introduced a mercury-free catalyst for the Dow Hyperlast Sub-sea Pipeline Insulation and Field-jointing series of polyurethane elastomers. These products has until recently been available with mercury catalyst only. The recently introduced Hyperlast™ Low Density Syntactic Polyurethane (LD512E) is now available only with non-mercury catalyst whilst the remainder of the Dow Hyperlast range of sub-sea products are now presented with the option

of non-mercury catalysts. According to the manufacturer it is without any loss of performance to their physical and chemical properties or to their hydrolytic resistance. (DOW, 2009)

A major supplier of bismuth/zinc based catalysts indicates that the industry is moving away from mercury catalysts and mercury catalyst is today not used in the development of new PU systems.

According to the trade organisations ISOPA and ALIPA, many companies have reformulated their PU systems because alternatives with the same performance as the mercury catalyst were not available (ISOPA, 2009).

Kometani *et al*. (year not indicated) from the Japanese chemical company Tosoh Corporation report that mercury catalysts are not used in Japan.

In some applications the mercury compound is also used as a biocide and in these applications it will also be necessary to add an alternative biocide.

C.6 Conclusion

A key feature of the socio-economic assessment has been consultations in order to understand the impact of the proposed restriction on different actors within the supply chain for phenylmercury compounds and their uses as catalysts in PU-systems (Part F). An overview of the number of stakeholders consulted and percentage of respondents are presented in Table G-1

As shown in Table G-1 all known EU manufacturers of phenylmercury compounds and formulators of catalysts have been consulted. A large part of the suppliers of alternative catalysts have also been consulted. The conclusion from the consultation with the suppliers of catalysts is, as stated above, that replacement of phenylmercury catalysts can be expected to be difficult for PU-systems representing about 30% of the total use of phenylmercury catalysts in the short term. At the same time the consultation has shown that the stakeholders expect to be able to replace all phenylmercury catalysts, without any loss of performance to their physical and chemical properties, given a transition period of 5 years.

It would have been useful to be able to consult a larger number of users of phenylmercury catalysts (formulators of two-component systems and producers of articles). Unfortunately, this has not been possible as the producers of these systems were not willing to give information about their customers due to commercial confidentiality.

This is however not essential when discussing alternatives to phenylmercury catalysts as it is the suppliers of catalysts that have the most extensive information about the different uses of the catalysts and will have the technological knowhow to develop alternatives.

So far we have not received any comments from industry during the extensive public consultation conducted by ECHA. In our opinion this supports the conclusions in this dossier.

The costs related to the substitution are discussed in part F of the dossier.

C.7 Other information on alternatives

No information.

D JUSTIFICATION FOR ACTION ON A COMMUNITY-WIDE BASIS

As part of the Community Strategy on Mercury, the European Commission proposed in 2005 that, in the medium to longer term, any remaining uses of mercury may be subject to authorization and consideration of substitution under the proposed REACH Regulation. In order to reduce EU demand, the remaining uses of mercury were also to be investigated and appropriate action taken, if needed.
There is an EU-level ambition to reduce the entry and circulation of mercury in society by cutting supply, because of the threat that mercury poses in the EU and on a global level. The justification for action is in the context of a widely recognized need to further reduce mercury emissions at an EU and global level.

D.1 Considerations related to human health and environmental risks

Mercury is considered a global persistent pollutant. Once released into the atmosphere, mercury can undergo long-range atmospheric transport. The global threat from mercury releases warrants action at local, national, regional and global level and there is a world-wide common effort to reduce demand and supply of mercury. This is well recognised by the Community Mercury Strategy and the UN Environment Governing Council. The life-cycle of the phenylmercury compounds leads to a significant release of mercury in the environment and adds to the overall emissions of mercury. Based on this, mercury use and releases from the phenylmercury compounds in the EU needs to be controlled on a Community-wide basis.

D.2 Considerations related to internal market

The proposed restrictions cover substances and articles that are traded between and are used in all EU Member States which has not yet established general restrictions on these products. The substances and articles containing phenylmercury compounds are both manufactured in and imported to the EU. The goods need to circulate freely within the EU. Regulating through Community-wide action ensures equal treatment for the producers and distributors of the substances and articles in different Member States.

D.3 Other considerations

UN has established an intergovernmental negotiating committee with the mandate to prepare a global legally binding instrument on mercury. The work is supported by the Council of the European Union. Acting at Community level, including the proposed restriction, also strengthens the EU efforts at the global level.

D.4 Summary

Action on a Community-wide basis is necessary for global persistent pollutants like mercury. Cross boundary human health and environmental problems will not be sufficiently controlled by national actions. The life-cycle of the phenylmercury compounds leads to a significant release of mercury in the environment and adds to the overall emissions of mercury. Regulating through Community-wide action ensures equal treatment for the producers and distributors of the substances and articles in different Member States. Based on this, mercury use and releases from the phenylmercury compounds in the EU needs to be controlled on a Community-wide basis. Acting at Community level, including the proposed restriction, also strengthens the EU efforts at the global level.

E JUSTIFICATION WHY A RESTRICTION IS THE MOST APPROPRIATE COMMUNITY-WIDE MEASURE

E.1 Identification and description of risk management options

E.1.1 Existing Community-wide risk management options

There is a range of current legislations that affect the use of the substances being proposed for restrictions. The most relevant current legislations are:

- Directive 2008/1/EC on integrated pollution prevention and control will apply to the manufacturers of the catalysts. Through permits laid out under this Directive, emission limit values and/or other technical parameters should be in place to limit emissions of mercury to the environment[17]. The European Commission has proposed a new Directive on industrial emissions which would replace this Directive. It is not expected that this will directly change the way that emissions of the phenylmercury compounds are controlled since emissions of these compounds are not predominantly from point sources. In addition, certain activities are not directly affected by IPPC. Annex 1 of Directive 2008/1/EC lists the production of basic plastic materials and production of synthetic rubbers as processes that fall under the scope of the directive. However, the specific production of PU-based articles using the mercury based catalysts such as production of sealants, coatings and adhesives is not listed in Annex 1 of Directive 2008/1/EC, this applies to the two thousand plus companies applying the mercury-containing PU systems. Moreover, emissions during the service life and the waste phase of these products will not be affected by this directive either.
- Under Directive 2000/60/EC (the Water Framework Directive), mercury and its compounds are classified as a priority hazardous substance. This means that measures need to be introduced to cease or to phase out releases to the water environment by 2025. In addition, an environmental quality standard has been agreed[18] that will limit the concentration of mercury allowed in the water environment from 2015. As river basin management plans are implemented over the coming years under this Directive, it is possible that additional measures will be required to reduce releases of the phenylmercury compounds to the environment. However, it is currently unclear whether these compounds are likely to be a significant focus of these management plans and it is not considered realistic to regulate emissions of phenylmercury compounds differently between river basins.
- The Hazardous waste directive (91/689/EEC) introduces a precise and uniform definition of hazardous waste and aims to ensure ecologically sound management of this waste flow. Mercury catalysed PU materials will typically contain the mercury compounds in concentrations in the range of 0.1-0.5%. In this concentration range, the waste of these materials would be classified hazardous according to the hazardous waste directive if the substances were classified very toxic, carcinogenic or mutagenic (EC, 2000). The phenylmercury compounds are in this concentration range not

[17] It is not clear whether the permits for the specific installations involved currently include emissions controls specific to the mercury-based substances

[18] 0.05 μg/l as an annual average and 0.07 μg/l as a maximum allowable concentration

classified toxic, carcinogenic or mutagenic and the waste materials are consequently not classified hazardous. Elemental mercury is classified very toxic (T+; R26) but the content of elemental mercury in the materials are considered to be below 0.1%. Waste of the catalyst product used for the formulation of the PU systems is classified hazardous, but the quantity of such waste is considered to be small. Furthermore emission during production and service life will not be affected by this directive. The Hazardous waste Directive has been incorporated and repealed by the new Waste Framework Directive (2008/98/EC) which sets the basic concepts and definitions related to waste management and lays down waste management principles.

- The waste incineration directive (2000/76/EC) places emission limit values on emissions of mercury and its compounds from installations incinerating waste. In particular, it includes a limit value for discharges of waste water from the cleaning of exhaust gases (0.03 mg/l) and an emission limit for air emissions of 0.05 mg/m3. Although this does not of course eradicate emissions from these sources it does limit the amount of mercury output from each incinerator installation. However, it is understood that the EU waste policy (Directive 2008/98/EC on waste (Waste Framework Directive)) will lead to increased incineration of waste. Therefore, it could be that limits on incineration exhaust gases would not lead to a limit on the total environmental release of mercury. Emissions during production, service life and land filling of these products will not be affected by this directive.
- Under the end of life vehicles directive (2000/53/EC), Member States are required to ensure that materials and components of vehicles put on the market after 1 July 2003 do not contain mercury, other than in (a) bulbs and instrument panel displays, (b) discharge lamps for headlight application, and (c) fluorescent tubes used in instrument panel displays. It is expected, therefore, that mercury should not be used in components such as gaskets, seals and other polyurethane systems (though the extent to which these have historically contained mercury is unclear). This directive does only affect vehicles. Emissions from other sources will not be affected by this directive.

E.1.2 Other Community-wide risk management options

- A possible sector-specific legislation is considered unsuitable because uses are varied and widely dispersed – it would be very difficult to apply and enforce to a large number of subsectors. Therefore the effectiveness of this type of legislation will be marginal.
- Voluntary industry agreement is another possible RMO. Although proportional in terms of cost to the industry, this kind of RMO will not be proportional to the risk. It will be very difficult to implement and enforce a voluntary agreement for imported articles as these products are not imported and used by a specific industry.
- As regards the REACH Authorization provision the phenylmercury compounds could potentially be identified as SVHCs based on Article 57 (f), equivalent concern, due to degradation/ transformation products with PBT-like properties. Article 57 (f) has not yet been used for identifying SVHCs. The time frame for the process of identification of the substances for the Candidate list, subsequent inclusion into Annex XIV and until the sunset date is reached would be comparable to the time frame before the proposed restriction enters into force. Authorization requires much administrative work, and imported articles containing the substances will not be regulated by

Authorization. Therefore, a restriction concerning imported articles would anyhow be necessary in addition to Authorization.

E.1.3 Proposed risk management options

Table E-3 at the end of this chapter provides an indicative qualitative scoring of the different risk management options. This is based on a simple appraisal of whether each of the options is likely to be suitable and the degree (high, medium, low) of suitability. In several cases the risk reduction capacity has been considered highly or moderately negative. That means that the risk management option is not suitable for the purpose. In these cases the risk management option has not been considered further. The following two risk management options are considered the most relevant as a means to reduce mercury emissions in the EU:

The primary restriction proposed (option 1) as outlined in Section A.1 of this document. In short it consists of a restriction of use, manufacture and placing on the market for the five phenylmercury compounds in question within 5 years after adoption (i.e. by start of 2018).

A secondary option has also been considered (option 2). This would require a phase-out over a shorter time period. For the purposes of this analysis, it has been assumed that this would be required over a period of two years (i.e. by start of 2015).

These two options have been discussed in more detail in Section E.2.

It is to note that RAC has proposed a slight change in the comparison of the different options: using the same “window” (from 2015, which may be the year of adoption of this restriction, to 2030, the year after which very probably a global ban will be implanted at the international level).

It is also to note that a third option has been introduced and discussed by RAC in its opinion: a 3-year delay for implementation. On a risk assessment point of view and especially as use follows an exponential decay, this restriction should be applied as soon as possible.
Both calculations are summarised in table E1 and E2.

E.2 Further assessment of proposed risk management options

In this section the two proposed restriction options are discussed using the main criteria effectiveness, practicality and monitorability.

E.2.1 Restriction option 1: Phase-out over 5 years

E.2.1.1 Effectiveness

E.2.1.1.1 Risk reduction capacity

In terms of the risk reduction capacity of this option:

- The restriction would remove all new use of the five compounds from the EU market within five years. This would lead to a consequent reduction in releases and exposure from all life cycle stages. However, exposure and release to the environment would continue to occur until the time that the restriction is implemented. In addition, releases of mercury from articles already in use would continue to occur until such time as they are removed from circulation. (The exposure assessment identifies releases during the service life as the single largest contributor to releases.)
- In terms of the potential alternatives likely to be used, as highlighted in Part C, it was concluded that these have significantly lower health and environmental effects compared to those containing mercury. However, if the substances in question are replaced by other mercury containing substances the risk reduction will most likely be marginal.
- This restriction would reduce releases to the environment and hence also reduce exposure. It is estimated that introduction of a restriction from the start of 2018 would reduce the total amount of mercury released to the environment by around 15 tonnes[19] in the first 10 years after implementation.

E.2.1.1.2 Proportionality

In terms of the proportionality of this option:

- Given that all life-cycle stages of the phenylmercury compounds lead to some releases to the environment, the restriction would be targeted to the identified risks and would not inadvertently affect actors in the supply chain which are not associated with the identified risk. However, the releases from manufacture of the phenylmercury compounds and the formulation of catalyst (as set out in the exposure assessment) are a very small proportion of the total EU-emissions (less than 0.01%).
- A restriction from which manufacture of the catalysts themselves was excluded would reduce the cost of the restriction. If we only consider risk reduction through lower emissions in the EU, this will make the restriction more proportionate. Nevertheless a restriction on manufacture may also reduce global emissions of mercury, and in that way also lead to a reduction in pollution problems associated with these substances as a result of long range transport of mercury. This issue will be addressed in more detail in Part F. As described in Section C.5, a restriction implemented over a period of 5

[19] Assuming releases to air and waste water as set out in Section B9.5.5 and an exponential decline in use under the baseline scenario based on historical changes in uses (with releases assumed to be proportional to use). The releases of mercury avoided are those that would otherwise have occurred over the period 2018 to 2037 from those products marketed after 2018.

years would allow virtually all of the current mercury catalyst use to be replaced. The calculations in Part F, show that the total cost of restriction option 1 is approximately € 9.7 million calculated as net present value, and the cost effectiveness is estimated to be 649 €/kg. Proportionality of restricting manufacture as regarding costs/benefits is also addressed in part F (see section F.2.10.2).

Based on the information above, it would appear that a restriction introduced over a period of 5 years would be proportionate in terms of technical feasibility and would not unduly penalize those firms operating in markets where substitution is more time-consuming[20]. In terms of economic feasibility, the cost of replacing systems using mercury catalysts is not expected to impose a significant cost to industry.

E.2.1.2 Practicality

Restriction option 1 is considered to represent an implementable option for the actors involved. As set out in Section C.5, it appears that the necessary technology, techniques and alternatives would be available and economically feasible within the timeframe of 5 years.

In terms of enforceability, the authorities would need to check compliance with the proposed restriction. The Member States should already have in place appropriate control systems with respect to enforcement, including effective, proportionate and dissuasive penalties for non-compliance. Relevant actors that may need to be included in enforcement of the restriction could include:

- Manufacturers of the phenylmercury compounds;
- Manufacturers of the catalysts containing the phenylmercury compounds;
- Importers of substances, mixtures and articles into the EU in order to check that the substances are not present and are not placed on the market (e.g. by customs officials).

There are other actors in the supply chains concerned, such as formulators of polyurethane systems and companies applying polyurethane systems. However, effective enforcement at the level of manufacturers and importers (of which there are currently far fewer than formulators and users of polyurethane systems) should be sufficient to address compliance with the restriction.

It is considered likely that enforcement of this restriction could be done within the remit of systems already in place for enforcement of existing restrictions.

Enforceability would potentially involve chemical analysis of the final article or checking that all steps have been taken by the article supplier to ensure that he has received the maximum level of information to be able to demonstrate that it complies with the restriction.

Similarly to enforcement, the manageability of the restriction would be mainly focused on those actors towards the top of the supply chain (i.e. manufacturers/importers of the compounds, catalysts and polyurethane systems). There are a small number of manufacturers of the phenylmercury compounds and the catalysts: fewer than four of each.

[20] It should be borne in mind that it has not been possible to consider all of the possible types of application that the PU systems may be used in within the context of this assessment. It is possible, therefore, that there may be some applications where substitution would be even more problematic and could not therefore be undertaken within a period of five years (for example, where use of specific PU systems based on the mercury compounds is specified in long-term contractual arrangements).

Assuming that replacement of the phenylmercury compounds is technically and economically feasible (see above) within the timescales of the proposed restriction, the restriction should be manageable for the downstream users.

Part of the consultation for this project attempted to find out from producers of polyurethane systems, the specific uses for which use of phenylmercury catalysts is essential and cannot be easily substituted. The essential uses that were indicated by firms consulted for this study were the repair of elastomers for use in extreme environments and in particular for use in the offshore oil and gas industry. Although it was possible to understand the key properties imparted to polyurethane end products by the use of phenylmercury catalysts, it was only possible to get an indication of the types of uses for which these products were essential.

In order to understand exactly how the PU products are used it would be necessary to consult with the customers of producers of polyurethane systems to obtain information on the specific uses of the products and the consequences of changes in key properties of the end products. Unfortunately, this was prevented by those consulted not being prepared or able to provide information on exact product use or give the contacts for their customers (because of commercial confidentiality). However, it is understood from one producer of polyurethane systems, that changes to end products from the use of systems without mercury catalysts would not, in their opinion, result in compromises to the safety of the use of the end products.

E.2.1.3 Monitorability

Monitoring implementation of this restriction could include a number of different aspects, such as:

- Determining/confirming that there is no remaining manufacture of the phenylmercury compounds or their use in production of catalysts. The number of current manufacturers is small, so this should not represent a significant additional burden for the authorities involved. It should be feasible to adapt existing mechanisms for monitoring of compliance with restrictions to cover these substances.
- In terms of imports of the substances to the EU, there is already a system for monitoring imports and exports of mercury compounds because of their inclusion under the Rotterdam Convention. As detailed in the section on manufacture and import (Section B.2), imports are included in the EDEXIM database. It should, therefore, be relatively straightforward to monitor any import of these substances into the EU.
- Because of current inadequacy of analytical methods to quantify the content of the phenylmercury compounds in PU-articles and the possibility that the compounds may be partly degraded in the articles, the concentration limit is proposed to relate to mercury. This is also in line with the EC regulation on cosmetic products (Regulation EC/1223/2009) where some mercury compounds, including phenylmercury acetate, are allowed for use as preservative. The concentration limit is 0.007 % (of Hg) and "If mixed with other mercurial compounds authorised by this Regulation, the maximum concentration of Hg remains fixed at 0.007 %". Another example is that in the US, there are processes in place for testing of polyurethane flooring to determine the mercury content in order to decide whether flooring removed from buildings should be

treated as hazardous waste due to the mercury content[21]. The analytical methods, and other analytical methods used for analysis for mercury in plastic materials with detection limits lower than the limit value proposed, are presented in Appendix 10. Analytical methods including sampling and preparation methods, for the phenylmercury compounds would be more problematic and must be further developed. It would not be feasible to attempt to sample all relevant polyurethane products but sampling could, for example, be undertaken for products where there is information to suggest that these substances are still being used. This would help to keep the administrative burden proportionate to the risks involved.

E.2.2 Restriction option 2: Phase-out over a shorter period

E.2.2.1 Effectiveness

E.2.2.1.1 1 Risk reduction capacity

In terms of the risk reduction capacity of this option:

- As with option 1, this option would remove all new use of the five compounds from the EU market but over a shorter timescale (assumed to be two years, from 2015 onwards), with a consequent reduction in releases and exposure of humans and the environment.
- In terms of the total mercury released, it is estimated that this option would reduce releases by around 18 tonnes in the first 10 years after entering into force in 2015 compared to around 15 tonnes under option 1.
- It is understood from the consultation that, in the event of a restriction being introduced, industry would be able to replace the majority (70% as described in Part C and F) of use of the phenylmercury compounds within 2-3 years. However, according to industry, there are a number of uses of these catalysts that would be problematic to Work is obviously already underway to develop and implement alternatives to the phenylmercury catalysts in polyurethane applications. However, requiring replacement within a shorter timescale could potentially mean that different choices are made regarding the alternatives that would be implemented in practice, potentially leading to different health and environmental effects. In theory, if substitution is required later (e.g. within 5 years), industry would have more time to ensure that the alternatives implemented are those that have substantially lower health and environmental risks, for example through more extensive information developed for compliance with REACH.

E.2.2.1.2 Proportionality

In terms of the proportionality of this option:

- This option will target the risk in the exact same manner as a restriction implemented over a longer time period (option 1).
- The considerations related to restricting manufacture of the phenylmercury compounds are the same as for option 1.

[21] MPCA (2008). Disposal guidance for mercury-catalyzed polyurethane flooring and subflooring. Minnesota Pollution Control Agency, Saint Paul.

- As described in Part C and F a restriction implemented over a period of 2-3 years would allow around 70% of the current use to be replaced. There are therefore a number of possible responses for those uses that could not be replaced within this timescale:
  - The products could be lost from the market and replaced with technically inferior alternatives (e.g. polyurethanes that do not have the desired characteristics). This could have implications for e.g. the frequency of replacement of articles in use and associated costs or for more frequent failure of articles.
  - Derogation for certain uses of the catalysts could be included, allowing a longer time for implementation in applications where substitution is most problematic. However we have not been able to establish which uses would need derogation.
- The calculations in Part F of this report indicate that the annual cost of restriction option 2 is around €14.6 million and the cost effectiveness 802 €/kg, using the method of net present value. In these calculations we assume that only 70 % of the mercury containing systems will be replaced within 2 years, substituting the remaining 30 % within 5 years after implementation (see Part F for the calculations). The administrative costs related to derogations are not included in these calculations. These could potentially be substantial.

Based on the information compiled for this study, it is considered likely that a restriction introduced over a period of 2 years could be disproportionate in technical and economical terms because there are indications to suggest that certain applications could not be replaced effectively within this timescale.

E.2.2.2 Practicality

There are potential concerns with the implementability of this option given that all of the actors involved would not be capable in practice of complying within a period of 2 years. This is because, for some applications (representing 30% of use), it is understood that the necessary alternatives would not be available within this timescale. There could, therefore, be an argument for having a step-wise approach, whereby the majority of uses would be restricted within a period of 2 years and the remainder (30%) within 5 years. However, the applications in which the catalysts are used are many and varied and, therefore, it is likely to be disproportionately resource-intensive to identify all of the applications that could be substituted within 2 years and all those that would require 5 years.

Consultation for this study suggests that the uses that could not be substituted within 2 years are for higher performance products for the repair of rubber components or linings for which there is heavy abrasion in use and/or for use in extreme environments (for example such as in the repair of elastomers in offshore applications in the oil and gas extraction industry). The main barriers to the substitution for these types of uses are technical and are associated with finding alternatives that can match the degree of cure and cure speed performance as well as the strength of the final product (for some uses consultation indicated that non-mercury containing substitutes resulted in products with 70% of the required strength, resulting in products not being fit for purpose).

In terms of enforceability, the exact same assessment as under option 1 applies. The issues related to the manageability of the restriction would be essentially the same as those for

option 1 (see above). However, the more time the industry is given to adapt to the restriction the easier it will be. Given that effective implementation of the restriction is likely to require communication on changes to product characteristics[22], there would obviously be less time for such communications to take place under this option. Similarly, if use of specific polyurethane systems is specified in long-term contracts, a period of 2 years would allow less flexibility to amend such contracts.

E.2.2.3 Monitorability

The issues surrounding monitorability of a restriction are likely to be exactly the same under this option as under a restriction implemented over a longer period.

E.2.3 Restriction option 3: Phase-out over a less short period (Alternative option introduced by RAC)

E.2.3.1 Effectiveness

E.2.3.1.1 Risk reduction capacity

Comparison of the different options with the baseline "business as usual".

The 2008 data and information from industry showed that 10 years ago volumes used were 2.5 times higher (industrial said between 2 and 3 times higher). DS then stated that the trend in use could be considered as an exponential decay and so compared option-1 (5 years implementation from adoption in 2012) and option-2 (2 years implementation from adoption in 2012) with the baseline corresponding to the possible mercury emissions that could be avoided during these periods. Estimations were that option-1 (5 years delay, period 2018-2027) would result in a reduction in mercury of 15 tonnes and option-2 (3 years delay, period 2015-2024) would result in a reduction in mercury of 18 tonnes.

According to RAC, several assumptions in these estimations could be seen slightly different:

a) Industry has stated that 2-3 years may be needed for substitution of 70% of the applications and that this may be more difficult. However, no delay supported by data was put forward for total substitution. Therefore it seems appropriate to compare with a third option, a 3 year delay. A shorter delay than 5 years is also considered relevant because as decay is considered to be exponential, the earlier the restriction is applied the more efficient it will be (quantities are much higher in the beginning of an exponential decay). The 2 years phase out might be too rapid forcing suppliers to just make a simple switch to other mercury-containing substances unless these are also restricted.

b) Considering the substitution difficulties, instead of a simple exponential decay one could consider the hypothesis of the addition of two exponential decays, a first one exactly as calculated previously but only for 70% of the uses, and a second one with a lower decay rate

[22] For example communication between catalyst suppliers and producers of polyurethane systems and between suppliers of polyurethane systems and end users. These may include, for example: communications regarding changes that may be required in incorporating the catalysts into the polyol components or possible differences in product application techniques that would require modified instructions for users.

constant to reflect the difficulties that may arise for 30% of the applications. This alternative for emissions predictions may increase the figures and thus underline a risk that the "natural decay" will take more time to end. RAC doesn't think that this refinement is needed, but wants to raise awareness on that DS emissions' predictions may be underestimated.

c) To compare the restriction options with the baseline, an end-of-emissions year if no risk management option is applied has to be fixed and calculations for all options adjusted to the same starting and end-of-emissions years. As end of 2012 the restriction may be adopted but the shorter option may only be implemented 2 years later, end of 2015 should be the starting-year to assess what may be the benefit of the different options. On the other end, considering on one side a "natural decay" that may end within 10 years (this means around 2021) and on the other side a global ban (possibly in 2018), a possible end-of-emissions year for calculation of the baseline could be 2020. However, two uncertainties can be introduced here: the natural decay could slow down slower if no external signal is given by authorities to industrials, and/or some derogations or delays could be introduced in UN's global ban. One should thus consider 2030 as a reasonable end-of-emissions year.

By applying all these modifications, estimations of the emissions and avoided emissions in EU can be calculated and summarised as indicated in the following tables E1 and E2 (these figures are recalculated with the same rules as DS used but by changing the starting and the end-of-emissions years):

Table E-1 Mercury emissions' predictions and comparison of the baseline "business as usual" with the different Restriction options.

n	Year	Phenylmercury-neodecanoate use (tonnes) Low	High		Max use t Hg		Hg emissions' predictions			
1	1998	90	175	Estimation relative to 2008 data (2.5×)	83	15.95				
2	1999	82	160	↓ Exponential decay hypothesis	76					
3	2000	75	146	↓ Tn: Tonnage prediction for year n	69					
4	2001	68	133	↓ T1: Tonnage of year 1998	63					
5	2002	62	121	↓ Rate constant: (year1/((year11-year1))*ln(T11/T1)	58					
6	2003	57	110	↓ ≈0.092	53					
7	2004	52	101	↓ Tn=T1*e^-0.092n	48	Max				
8	2005	47	92	↓	44	emission				
9	2006	43	84	↓	40	t Hg				
10	2007	39	76	↓	36					
11	2008	36	70	provided data	33	6.38	Hg emitted / Hg use ratio			0.191
12	2009	33	64		30	5.80	Baseline	Restriction options		
13	2010	30	58		28	5.29	0	2	3	1
14	2011	27	53		25	4.82	business as usual	2-year	3-year	5-year
15	2012	25	48	Restriction adoption (end of this year)	23	4.40				
16	2013	23	44		21	4.01				
17	2014	21	40	Option-2 = 2 years for implementation	19	3.66				
18	2015	19	37	Option-3 = 3 years for implementation (RAC's proposal)	17	3.34	3.3	3.3	3.3	3.3
19	2016	17	33		16	3.04	3.0	3.0	3.0	3.0
20	2017	16	30	Option-1 = 5 years for implementation (DS proposal)	15	2.78	2.8	2.8	2.8	2.8
21	2018	14	28		13	2.53	2.5	2.5	2.5	2.5
22	2019	13	25		12	2.31	2.3	2.3	2.3	2.3
23	2020	12	23		11	2.11	2.1	2.1	2.1	2.1
24	2021	11	21		10	1.92	1.9	1.9	1.9	1.9
25	2022	10	19		9	1.75	1.8	1.8	1.8	1.8
26	2023	9	18		8	1.60	1.6	1.6	1.6	1.6
27	2024	8	16		8	1.46	1.5	1.5	1.5	1.5
28	2025	8	15		7	1.33	1.3	1.3	1.3	1.3
29	2026	7	13		6	1.21	1.2	1.2	1.2	1.2
30	2027	6	12		6	1.11	1.1	1.1	1.1	1.1
31	2028	6	11		5	1.01	1.0	1.0	1.0	1.0
32	2029	5	10		5	0.92	0.9	0.9	0.9	0.9
33	2030	5	9	UN global ban may enter into force	4	0.84	0.8	0.8	0.8	0.8
							Emitted	29.3	0.0	3.3	9.2
							Avoided	0	29.3	25.9	20.1

Table E-2 Summary of Table E-1to highlight the comparison of the emissions and avoided emissions between baseline "business as usual" and the three different implementation delays proposed for Restriction of the five phenylmercury compounds.

Tonnes mercury	**from 2015** (implementation of the shorter delay restriction option) **until 2030** (global mercury ban)	
	Emitted	**Avoided emissions**
Baseline "**business as usual**"	**29.3**	**0.0**
"Option-1" **5-year delay**; proposed by DS	**9.2**	**20.1**
"Option-3" **3-year delay**; proposed by RAC	**3.3**	**25.9**
"Option-2" **2-year delay**; used by DS for comparison with option-1	**0.0**	**29.3**

When comparing the different delay options of this Restriction with the emissions' baseline ("Business as usual") it has to be underlined that implementation should take place as soon as possible to provide a real benefit in term of avoided risks: if the 2-year-delay is not chosen, one additional year (option-3) will lead to 11% more mercury emissions, and 3 additional years (option-1) will lead to as much as 31% more mercury emissions.

E.2.3.1.2 2 Proportionality

Analysis is similar to the 2-year delay option (option-2) except that 3 years correspond to the upper limit to guarantee 70% substitution. In addition:
As numerous identified alternatives which may exhibit less risk were already applied, and as RAC considers that there are high uncertainties regarding the delay needed to put in place all alternatives (the only indication is 70% substitution within 2-3 years and no data states the improvement in term of substitutions if delay is extended from 3 to 5 years), the option-3, a total ban within a 3-year delay, appears to be the most appropriate risk management measure from a risk assessment point of view.

From a socio-economic point of view, no information on costs and other consequences of a 3-years phase out period (e.g. substitution by the easiest available alternatives which might be other organo-mercury compounds) is available in order to conclude on the proportionality of such an option. Consultations with industry showed that 70 % of the mercury-containing PU systems can easily be replaced within 2 – 3 years; the remaining 30 % would be more difficult and need further R&D activities. It is expected that substitution for those 30 % is possible after 3 – 5 years which leads to the conclusion that the 5 years option seems to be the most appropriate risk management measure from a socio-economic point of view. No information in order to conclude on the proportionality of restriction option 3 (phase-out period of 3 years) is available.

E.2.3.1.3 Practicality

Analysis is similar to the 2-year delay option (option-2) except that 3 years correspond to the upper limit to guarantee 70% substitution. In addition:

As numerous identified alternatives which may exhibit less risk were already applied, and as RAC considers that there are high uncertainties regarding the delay needed to put in place all alternatives (the only indication is 70% substitution within 2-3 years and no data states the improvement in term of substitutions if delay is extended from 3 to 5 years), the option-3, a total ban within a 3-year delay, appears to be the most appropriate risk management measure from a risk assessment point of view.

From a socio-economic point of view, there are concerns as far as the implementability of this option is concerned given that industry indicated that not all applications can be replaced within a period of 3 years. For about 30 % of the applications the necessary alternatives might not be available within a shorter timeframe than 5 years (see section E.2.3.1.3 above). From a socio-economic point of view, therefore, a restriction with a 5 years phase-out period is regarded to be the most appropriate risk management option.

E.2.3.1.4 Monitorability

The issues surrounding monitorability of a restriction are likely to be exactly the same under this option as under a restriction implemented over a longer period.

E.2.4 Comparison of the proposed restrictions

Two options have been considered by the dossier submitter, involving the possible restriction entering into force either five (option 1) or two years after its assumed adoption (option 2).

In terms of a comparison of the two restriction options, the risk reduction capacity of option 1 is 31% less than that of option 2 because the restriction would be implemented three years later. There would therefore be greater emissions under option 1 (those related to new uses between 2015 and 2018).

Option 2 would be less proportionate and more difficult to implement than option 1, because the necessary alternatives are not expected to be available for certain applications within a shorter timescale. This could lead to substantial difficulties in substituting all of the uses, leading to greater costs and also potentially to unforeseen consequences associated with the end uses in which the polyurethane systems are applied. Consultations have indicated that substitution is feasible within 5 years after adoption.

The enforceability and manageability of option 1 is greater than that of option 2 because of the time needed for authorities and industry to adequately prepare for the restriction. It is considered to be no substantial difference in the ability of those involved to monitor the effectiveness of the two options.

Although option 2 – a restriction introduced over a two-year period – is likely to lead to a greater overall reduction in releases of mercury to the environment than option 1, it is the conclusion of the current assessment that option 1 would be the preferred option of the two. This is because there is evidence from the industry using the substances that there would be technical difficulties in replacing the substances over a period shorter than five years, although probably not for all uses. In order to avoid the potential unforeseen consequences of a restriction over a shorter period, it would seem prudent to allow sufficient time for the

replacement of these substances to take place. There is insufficient information available to determine how a stepwise phase-out of the substances could be achieved so the impacts of such an approach have not been investigated in depth.
A third restriction option has been introduced by RAC, which proposes an entry into force of the restriction after 3 years of its adoption. The conclusion is that from a risk reduction point of view, this option is the most appropriate risk management measure.
From a socio-economic point of view no information on costs and other consequences of a 3 years phase-out period is available and therefore it is not possible to draw any conclusion on the socio-economic consequences of option 3.

E.3 Summary and comparison of risk management options discussed

A number of different risk management options have been considered. Based on the arguments above, it has been concluded that current legislation is not sufficient to regulate emissions from the manufacture and use of the substances, and that a restriction is the best option.

Table E-3 below provides an indicative qualitative scoring, produced by the dossier submitter, of the different risk management options against each of the criteria and parameters. This is based on a simple appraisal of whether each of the options is likely to be suitable and the degree (high, medium, low) of suitability.

Table E-3 Assessment matrix for risk management options against three key criteria

	Effectiveness		Practicality			Monitorability			Overall
	Risk reduction capacity	Proportionality	Implementability	Enforceability	Manageability	Availability of indicators	Ease of monitoring	Availability of monitoring mechanisms	
Restriction option 1	++	++	++	++	++	++	++	++	++
Restriction option 2	+++	-	-	+	+	++	++	++	++
IPPC	--	x	x	x	x	x	x	x	--
Waste legislation	---	x	x	x	x	x	x	x	---
Water Framework Directive	---	x	x	x	x	x	x	x	---
Sector specific legislation	---	x	x	x	x	x	x	x	---
Voluntary agreement	--	x	x	x	x	x	x	x	-
REACH Authorisation	+	++	-	++	++	++	++	++	+

Key to assessment of suitability of options:

+++ highly positive ++ moderately positive + marginally positive

--- highly negative -- moderately negative - marginally negative

X not considered further.

F SOCIO-ECONOMIC ASSESSMENT OF PROPOSED RESTRICTION

The socio-economic analysis performed in this section is based on the information described earlier in the dossier. Some information has been attained through additional consultation with industry conducted mainly for the purpose of this analysis. Appendix 4 contains a summary of the socioeconomic impacts that have been considered.

F.1 Estimates of expected future releases to the environment

Section B.9 of this dossier provides estimates of releases of the mercury compounds to the environment, based on current production and use levels (data relate to 2008). Table B-60 shows estimates of future baseline emissions (no restriction). Based on these numbers it was estimated the emissions avoided trough a restriction both with a short (2 years) and a long (5 years) phase-out period.

Table F-1 Summary of emissions avoided through option 1 and option 2 (tonnes Hg – not including articles) (see also alternative way proposed by RAC to compare the different options in table E1)

Years after entering into force	Option 1 (2018-2027)	Option 2 (2015-2024)
1	1,2	1,1
2	1,3	1,2
3	1,4	1,3
4	1,6	1,8
5	1,7	1,9
6	1,8	2,1
7	1,7	2,0
8	1,5	1,9
9	1,4	1,8
10	1,3	1,7
Total emissions avoided over assessment timescale)	15	17
Average annual emissions avoided from when restriction takes effect	1.5	1.7

There could be significant emissions avoided through a restriction, estimated at around 15 tonnes in the first 10 years after implementation of option 1 and 17 tonnes the first 10 years after implementation of option 2. These figures are lower than the annual potential release quoted in Section B.9. The main reason for this is the lifespan of products and gradual release of mercury from the products in use and in the waste phase. This is described in more detail in Section B.9. It is also important to point out that the avoided emissions quoted above do not include avoided emissions from imported articles or potential reductions in emissions outside the EU. The potential avoided emissions from imported articles might be significant, but it has not been possible to quantify these emissions.

For the purpose of providing an indicative estimate of the likely future releases to the environment that could be avoided through a restriction the following approach has been taken:

- It is assumed that use of the substances will decline in line with the baseline estimates provided in Section B.9.
- It is assumed that the average product lifetime is 5 years
- For service life emissions, emissions in 2018 are assumed to be based on the releases from those products that enter into use in that year. This is based on the 'steady state' emission estimate for 2008 (3.01t), multiplied by the proportion of 2008 use in 2018 (0.40), multiplied by 1/5 to take into account that the 2008 emissions are based on a steady state and assuming that the 5 year lifetime applies, giving emissions of 0.24t. Likewise, emissions in 2019 are then based on the second year's emissions from products entering into use in 2018 (0.24t) plus emissions from products entering into use in 2019, which is again based on the 2008 emissions (3.01t), multiplied by the proportion of 2008 use in 2019 (0.36) and by 1/5, giving 0.22t + 0.24t = 0.46t. This process is continued for subsequent years, with emissions in each year comprised of releases from products entering into use over the preceding 5 years. For emissions in 2018 to 2021, releases from products entering into use prior to 2018 are not included because they would not be directly affected by the restriction.
- Emissions from waste incineration are based on the emissions in 2008 (0.75t) multiplied by the fraction of 2008 usage. It is assumed that products will not enter the waste phase and hence be incinerated until after five years (the assumed product lifetime), such that emissions in 2023 are based on the fraction of 2008 use that occurs in 2018 (0.40) multiplied by 0.75t, to give 0.30t.
- Emissions from landfills in 2008 are, in the exposure assessment, calculated to be 0.25t over a period of 20 years. Therefore, if a steady state were to apply, annual emissions would be 0.25t, relating to products landfilled over the previous 20 years (i.e. 0.015t for the quantities landfilled in each year). This is based on an emission factor of 0.01 and the amount assumed to be disposed of to landfill (25.16t).
- For the purposes of this analysis, emissions from landfills are assumed to occur with a 5 year lag due to the assumed service life of the products. Thus, products entering into use in 2018 will be landfilled in 2023. So, emissions in 2023 are 1/20 of those related to use in 2018 (which is 0.40 as a fraction of 2008 use), i.e. 0.40 multiplied by 0.25t as the 2008 steady state value multiplied by 1/20 = 0.005t. Then, in 2024, emissions are 1/20 of those related to use in 2018 (0.005t) plus the same for use in 2019 (0.36 x 0.4t x 1/20 = 0.005t), giving a total of 0.010t. Emissions related to use in years prior to the restriction (2018) are not included because they would not be affected by the proposed restriction.
- For restriction option 2 it is assumed that 70 % of the systems, and consequently 70 % of the emissions will be substituted in 2015 and the remaining 30 % will be substituted in 2018. The reason for this is the information attained from industry which indicates that it will only be possible to substitute 70 % of the mercury containing catalysts within 2 years. This is discussed in more detail in Section C.5.

In broad terms, emissions are assumed to decline due to the decline in use of the substances in the EU over time. The estimated emissions do not include release from imported articles containing the substances. Emissions from imported articles will take place during service life and waste disposal and it is expected that the decline in releases from use of imported articles will be less pronounced. However, no quantitative data are available on imports of articles, and hence emissions. As a result of this these emissions are not included in the assessment.

Using this approach, an estimate of the emissions of mercury that could be avoided the first 10 years after a restriction that takes effect in 2018 (option 1) and 2015 (option 2) have been estimated to be as shown in the table F.1. These represent all of the emissions in the EU that are likely to occur from the phenylmercury compounds that enter into use after 2018 and 2015 respectively.

A fairly large amount of mercury will end up in landfills. Some of this will be released to the environment during the time span of 20 years. This amount is included in these estimates. The rest of the mercury will accumulate in the landfills and remain there beyond this period. This has a potential for release to the environment at a later stage. This amount is not included in these estimates. Release to the environment from landfills is discussed in Section B.9.

F.2 Economic impacts

F.2.1 Compliance costs

The analysis undertaken by Cowi and Concorde East/West (2008) indicated that, in 2008, there were as many as 200 to 250 different mercury-catalysed PU elastomers (MCPUE) systems across the EU. For the purposes of this study, it is assumed that in the beginning of 2008 there were 250 MCPUE systems.

As indicated in Section C.5 it is believed that 70% of these systems could be replaced with mercury-free systems within 2 years (i.e. 175 systems), whilst the remaining 30% (i.e. 75 systems) would be more difficult to replace, and may require additional time (e.g. 5 years).

During the work on the SEA of this restriction the suggested numbers were double-checked with industry and there were no indications to suggest these numbers are incorrect, see Part G. In addition, no comments have been received from industry, during the public consultation for the proposed restriction so far, to suggest these numbers are incorrect. It is assumed that the number of MCPUE systems under the baseline scenario would reduce at a rate proportional to the assumed reductions in mercury consumption (tonnes) as described in B.2. This is set out in the table F.2 and figure F.2 below.

If a restriction is imposed, it would require industry to replace MCPUE systems with mercury-free systems. This is expected to be the main (net) cost impact upon industry. According to information from industry the main cost of finding a suitable alternative system for customers would be R&D costs. This cost would also be passed through in the prices of systems sold.

The numbers are based on the restriction being adopted at the end of 2012. Therefore under restriction option 1, the restriction would apply from January 2018 and under restriction option 2, the restriction would apply from January 2015.

Very little information is available related to the quantum of imported articles containing phenylmercury. As a result of this the costs for imported articles are not included in the cost calculations in this section. It is however expected that these articles are the same category as those produced in the EU. As a result of this it is expected that the costs related to the restriction on imported articles would be of the same magnitude for the users as the cost for articles produced in the EU.

Table F-2 Assumed number of MCPUE systems over time (end of year) under the baseline scenario

Beginning of the Year	Number of systems still using mercury catalyst under baseline scenario
2008	250
2009	228
2010	208
2011	190
2012	173
2013 (restriction adopted)	158
2014	144
2015 (entry into force of restriction option 2)	132
2016	120
2017	110
2018 (entry into force of restriction option 1)	100
2019	91
2020	83
2021	76
2022	69
2023	63
2024	58
2025	53
2026	48
2027	44
2028	40
2029	36
2030	33

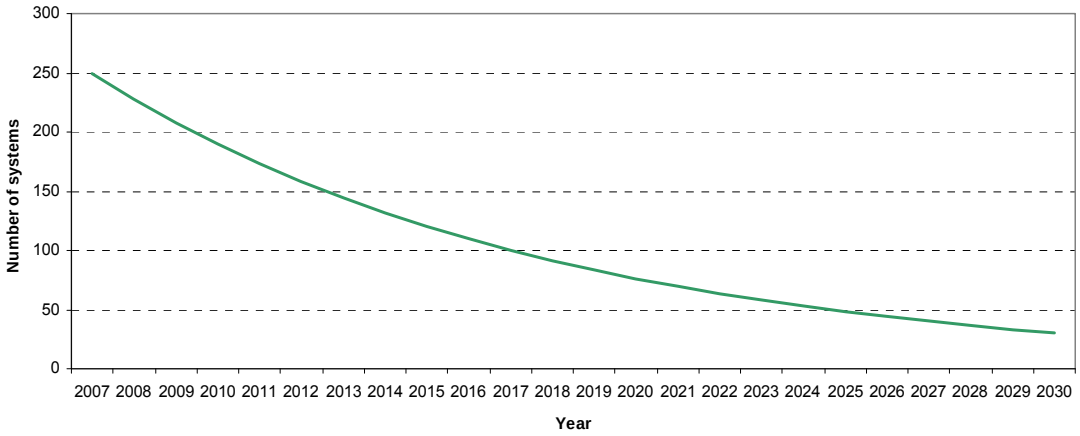


Figure F.2-1 Assumed number of MCPUE systems over time under the baseline scenario

The number of systems that would need to be replaced in the absence of a restriction will vary depending on the restriction option chosen. This is set out in Table F.1. Under restriction option 1 (phase out in 5 years), in 2013 there are expected to still be 158 MCPUE systems. By the beginning of 2018, in the absence of any restriction there would still be 100 MCPUE systems. If a restriction is adopted, then the compliance costs will be the costs of replacing 100 systems by the beginning of 2018.

Under restriction option 2 (phase out in 2 years) again by 2013 there will still be 158 MCPUE systems. By the beginning of 2015, in the absence of any restriction there would still be 132 MCPUE systems. If a restriction is adopted, then the compliance costs will be the costs of replacing 132 systems by the end of 2015, summarised in Table F.3, below.

It is assumed that any reductions in MCPUE systems under the baseline scenario relate to those MCPUE systems where it is "relatively easy" to substitute with an alternative mercury free system. It is thought that around 30% of MCPUE systems available in 2008 (i.e. 75 systems) would be difficult to replace. It is considered reasonable to assume that any reductions in the absence of a restriction would relate to those MCPUE systems where it is easier and less costly to switch to an alternative. Therefore, it is assumed that the most difficult systems (totalling 75) will be the last to be replaced.

In the calculation of cost and emissions avoided for restriction option 2 it is assumed that only 70 % of the systems in use by the beginning of 2015 can be substituted this year. The remaining 30% (i.e. 40 systems) are assumed not to be substituted until 2018[23]. As a result of this it is assumed that derogations will be granted for a number of systems in this period (2015-2018).

Table F-3 Assumed number of systems that need to be replaced under the two restriction options

Proposed restriction options	Number of MCPUE systems (by the start of the restriction)	Number of systems which can be relatively easily substituted to a Hg free system	Number of systems where it will be difficult to substitute
Proposed restriction option 1 (Phase out in 5 years)	100	25	75
Proposed restriction option 2 (Phase out in 2 years)	132	57	75

Based on the study by Cowi and Concorde East/West (2008), it is estimated that the one-off cost of Research & Development will vary depending on the time given to industry to find a suitable mercury-free alternative. If 5 years were given, COWI and Concorde East/West (2008) reports that the industry considers a "relatively easy" substitution, to be defined as research carried out by one (equivalent) researcher over 7-8 weeks, plus overhead and materials, for a total of some €10-15 000. Alternatively, a more challenging substitution might imply research and development costs of €25-40 000.

[23] For the remaining 40 systems not substituted until 2018 unit cost numbers are the same as the ones used for substituting difficult systems in restriction option 1.

If the time period were reduced to 2 years, it is assumed this would add a premium of 40-50% due to more resources being used to search for substitutes rather than developing new systems for new products. The one-off costs used in the analysis are shown in the table below. This information was confirmed in the consultations performed for this analysis.

Table F-4 One-off R & D costs (per system) associated with switching to Hg free alternatives

Restriction options	Unit costs of systems which can be relatively easily substituted with a Hg free system		Unit costs for systems where it will be difficult to substitute	
	Low	High	Low	High
Restriction option 1 (Phase out in 5 years)	€ 10 000	€ 15 000	€ 25 000	€ 40 000
Restriction option 2 (Phase out in 2 years)	€ 14 000	€ 22 500	€ 35 000	€ 60 000

Note: All one-off costs can in principle be spread over the phase-out period.

In the calculations below, we use the high cost estimates only to reduce the risk of underestimating the costs.

Using this information, it is estimated that the total one-off R & D cost (at the EU level), using a phase-out period of 5 years (restriction option 1), is around €3.4m, assumed paid in full the year the restriction takes effect (2018). The expected economic lifetime of the investment[24] is assumed to be 10 years.

If a shorter (2 year) phase-out period is used (restriction option 2), then the total one-off cost of compliance (at the EU level) is estimated to be €5m. The majority of this cost is assumed paid in 2015 (the cost of replacing the 70 % of the systems) and the remaining cost paid in 2018.

Table F-5 R & D cost– Restriction options

	Total one-off cost of R & D (€m)	Net present value (2010 €m)
Restriction option 1 (Phase out in 5 years)	€ 3.4m	€ 2.4m
Restriction option 2 (Phase out in 2 years)	€ 5.0m	€ 3.8m

Note: Net present value figures are based on a 4% discount rate as set out in the SEA guidance and EU Impact Assessment guidance

This is the R & D cost of substituting the mercury-containing systems used in the EU by restricting use and placing on the market of the 5 phenylmercury substances. To assess the socio-economic impact of restricting use and placing on the market without restricting

[24] We take a conservative approach to the economic lifetime of the investment in R & D. The 10 years chosen is an assumption on how long the average alternative catalyst, developed as alternatives, will be marketed. This is a considerably shorter marketing lifetime than the existing Hg-containing catalysts. The reason for choosing a shorter time span is the perception of a more fluent and dynamic market with greater competition between different catalysts.

manufacture, the R & D costs can be assessed separately from the cost of lost export presented below.

F.2.2 Sunk costs

A consequence of introducing a restriction is that the benefits of investment already spent (e.g. R&D and testing) by industry using MCPUE systems may not be fully realised due to a premature end to the use of MCPUE systems containing the phenylmercury compounds. This potential loss of return on investment would be more significant with a shorter phase-out period. According to Cowi and Concorde East/West (2008) the capital used in manufacturing and formulating Hg–containing catalysts can be used to manufacture alternative catalysts as well. This is expected to contribute to a reduction in potential sunk costs.

F.2.3 Loss of export revenue

Manufacturers and users of the mercury compounds would see a premature end to their sales and associated revenue. This could also lead to loss of employment. Those that will be particularly affected will be manufacturers who predominately export the mercury compound outside of the EU (e.g. manufacturers of phenylmercury neodecanoate, phenylmercury acetate and phenylmercury 2-ethylhexanoate). This market might be lost to competing mercury manufacturers outside of the EU, rather than users necessarily switching to a mercury-free compound.

Based on informal consultation with such producers, it is understood that they do not envisage being in the market for the foreseeable future. Therefore, a restriction would accelerate closure of that part of the business, rather than giving incentives to a switch to producing mercury-free substances. Even if the restriction only banned the placing on the market of these mercury compounds, manufacturers have argued that the export market is not sufficiently large to continue operations, as without the EU market, there will be higher costs of raw materials (upstream costs) since they would not be buying in bulk. Therefore it would not be profitable to continue manufacturing to sell to a small export market only.

As an estimate of the annual loss of revenue from exports, using 2008 data, between 94[25] - 194[26] tonnes of mercury compounds were exported, with a sales value of around €45/kg[27] . The total sales revenue from exports in 2008 would thus have been around €4.3m – €8.7m. Information from industry indicates a falling baseline in the amount exported. A manufacturer of phenylmercury substances indicated that production would not continue beyond 2013 because of a global decline in the market for phenylmercury substances. Therefore there might not necessarily be any loss of revenue by the time a restriction is in place.

Assuming exports follow the same baseline as use in the EU, presented in Section B.2, the present value (€ 2010) of the cost of lost exports is estimated to be around € 10.8 million for restriction option 2 and € 7.3 million for restriction option 1. The socio-economic cost of lost export is the producer surplus, or value added, lost to European producers/exporters. In lack of any indications of cost structure a linear 45 degree marginal cost curve has been assumed

[25] 5t of Phenylmercury acetate, 49t Phenylmercury 2-ethylhexanoate, 40t Phenylmercury neodecanoate
[26] 10t of Phenylmercury acetate, 99t Phenylmercury 2-ethylhexanoate, 85t Phenylmercury neodecanoate
[27] Range of €40-50/kg - Options for reducing mercury use in products and applications and the fate of mercury already circulating in society, Final Report by COWI A/S for the European Commission, December 2008

to extract the producer surplus from the revenue. The socio-economic cost is therefore calculated to be about half of the export revenue.

The loss of export is due to the restriction on manufacture and not the restriction on use. To assess the impact of including manufacture in the restriction the cost of lost export can be assessed separately from the cost of R & D presented above.

F.2.4 Redistribution of EU sales revenue

For manufacturers and users of mercury compounds with predominately EU- based customers, it is possible they will switch to manufacturing and using a mercury-free process. Alternatively their sales will be displaced by increases in sales for existing manufacturers and users of mercury-free compounds and potentially increased employment in those firms. Therefore, some of these impacts could simply be redistributed rather than actually being a loss in output from an EU-wide perspective, especially with a restriction that bans the imports of articles containing these mercury compounds.

F.2.5 Operating costs to users

For many uses there already, or will relatively soon, exist alternative mercury-free compounds. The market is already dominated by mercury-free compounds (>95% of the market). Therefore there may not be any significant welfare losses from loss of choice of products on the market. There may however be some niche uses where it is more difficult to substitute to a mercury-free alternative (e.g. cost and/or time required) and there maybe some initial welfare losses from such as loss of durability in these alternatives. Based on consultation with industry and trade associations, the only uses specifically mentioned as being possibly problematic to replace in the short term were those for uses in extreme environments, such as the oil and gas industry. We have not been able to identify any specific products where substitution will be especially difficult during the public consultation so far. However, the diverse and numerous uses make it difficult to be certain that there will be no significant loss of functionality or durability for any products.

There is expected to be minimal avoided operating costs from using an alternative mercury-free system. Catalyst producers could potentially benefit from a reduction in waste disposal costs, as they will no longer have to deal with disposal of hazardous waste, arising from residual use when mixing mercury containing two-or-three-part systems. This is not expected to be significant.

F.2.6 Administrative costs

Users will initially incur some search costs associated with finding a suitable alternative and "menu" costs from trying to find an inexpensive and reliable supplier. This is unlikely to be significant and is already encompassed in the one-off R&D cost provided by industry from the COWI report[28] .

There will however be some additional monitoring, compliance and enforcement costs to competent authorities to check that imports of substances are not occurring and that there are no imports of articles containing these phenylmercury substances. If a system to grant derogations will be needed the administrative costs will increase substantially. There will be a

[28] Clarification obtained from original authors.

need for such a system if restriction option 2 (short phase-out period) is to be implemented without losing the performance of the products.

F.2.7 Cost per kilogram of the two restriction options

When calculating the cost-effectiveness of the two restriction options, we use the period between 2010 and 2028 as the assessment period. The restriction will of course have effect for a longer period than this, but an analysis timeframe is necessary for doing the calculations. The reason for assessing the two options over this period is that all substitutions under the two alternatives will have an economic lifetime until 2028 or earlier. For restriction option 1 all systems will be substituted in 2018 and are assumed to remain in the market for the subsequent ten years (end of 2027). For restriction option 2, 70% of the systems will be substituted in 2015, and are assumed to remain in the market for the subsequent ten years (end of 2024[29]). The remaining 30 % will be substituted in 2018 and are assumed to remain in the market for the subsequent ten years (end of 2027).

If use continues to decline as predicted under the baseline scenario, the total reduction in emissions during the assessment period is estimated at:

- 15 tonnes under restriction option 1 (5 year phase-out)
- 17 tonnes under restriction option 2 (2 year phase-out)

Using the costs of restriction (compliance plus loss of revenue from exports), it is possible to estimate an approximate cost per kg of mercury reduced. This is shown below:

Table F-6 Cost* per kg Hg avoided (€/kg)

	Net present value 2010 € million	Total emissions avoided kg	Cost per kg (€/kg)
Restriction option 1	€ 9.7	14 900	€ 649
Restriction option 2**	€ 14.6	18 211	€ 802

*Costs related to replacing articles are not calculated.

** The costs to users, alternatively the administrative costs related to derogations, are not included in these calculations. These could potentially be substantial.

The cost per kg may be seen as significant but the costs need to be compared to the benefits of the restrictions[30]

As stated throughout the dossier it has not been possible to quantify the amount of mercury-containing PU articles imported into the EU. As a consequence it has not been possible to quantify the cost of, or the reduction in emissions from, restricting imported articles. However, it is likely that this, through possible increased price on imported articles, would lead to a cost-effectiveness ratio in the same order of magnitude as that calculated above. The reasoning behind this is that we do not expect higher costs related to developing suitable alternatives outside the EU than within. And, if this is not the case, foreign producers of PU

[29] Costs and benefits are only calculated for the initial substitution, as renewal of product portfolio is assumed to be conducted regardless of the imposition of a restriction.

[30] One should bear in mind that the costs are discounted and the emissions avoided are not. This means that restriction option 2 will appear slightly worse relative to option 1 than it is in reality. This is because both costs and benefits will come sooner than in option 1.

systems will be able to import the alternative catalysts from the EU. Therefore we believe it is a fair assumption that the cost-effectiveness of prohibiting articles containing the 5 Phenylmercury compounds will not alter the cost-effectiveness of the restriction dramatically.

F.2.8 Assessment of restricting manufacture and use separately

To assess the impact of including manufacture in the restriction we have done additional calculations for restriction on use and manufacture separately as presented in F.2.1 and F.2.3. The cost effectiveness (€/kg) of restricting manufacture and use separately is presented in the table below.

By not restricting manufacture the cost of the restriction would be reduced considerably as there will no longer be a loss of export. However, as stated above there is a possibility that exports will cease anyway. Manufacturers have argued that the export market is not sufficiently large to continue operations. Without the EU market there will be higher costs of raw materials (upstream costs) since they would not be buying in bulk. Therefore it would not be profitable to continue manufacturing to sell to a small export market only.

The reduction in emissions in the EU would be virtually the same as the emissions from manufacture of the 5 phenylmercury compounds are negligible. The cost of restricting use and placing on the market only would be € 2.4 million for restriction option 1 and € 3.8 million for restriction option 2 in net present value (2010 €). Divided by the reduction in Hg emissions in the EU the cost-effectiveness is estimated at 159 €/kg for restriction option 1 and 209 €/kg for restriction option 2. The assessment period and calculations are the same as in F.2.7, the only difference is that the cost of lost export is excluded.

The benefit of restricting manufacture depends on the degree of substitution outside the EU. If the reduction in exports is replaced by mercury-containing catalysts produced outside the EU, there will be no benefit in restricting manufacture. Hence the cost-effectiveness will approach infinity. Alternatively, the mercury-containing catalysts exported from the EU will be substituted with mercury-free alternatives (possibly imported from the EU) and the global emissions of mercury will be reduced. The most likely scenario is probably somewhere between these two alternatives. Reducing global emissions could benefit the EU by reducing the global pool of mercury which could lead to lower long range transported pollution of mercury in the EU.

Using the same release factors that were used for calculating emissions in the EU, presented in Section B.9, restricting manufacture could potentially reduce the emissions outside the EU between 2010 and 2028 by up to 46 tonnes Hg for restriction option 1 and up to 56 tonnes Hg for restriction option 2. We have assumed the same declining baseline as for the use and emissions in the EU[31] . The potential for reductions in emissions are large, however to what extent substitution actually will take place is highly uncertain.

If we assume that all the exported catalysts are substituted with mercury-free alternatives and the subsequent reduction in emissions of mercury are calculated using the same release factors as for the calculation of emissions in the EU, the cost-effectiveness for the EU of reducing the global emissions of Hg is approximately 158 €/kg for restriction option 1 and 192€/kg for restriction option 2. As a full substitution is highly unlikely, the cost-effectiveness ratio would probably be less favourable than this.

[31] Calculations shown in appendix 11

In Table F-7 the different calculations of cost effectiveness are presented to ease the comparison of the result.

Table F-7 Summary of cost estimates*

	Restricting use and placing on the market		Restricting manufacture		Proposed restriction	
	Cost million € 2010	Cost effectiveness	Cost Million € 2010	Cost effectiveness	Cost Million € 2010	Cost effectiveness ***
Restriction option 1	€ 2.4	€/kg 159	€ 7.3	€/kg >158	€ 9.7	€/kg 649
Restriction option 2**	€ 3.8	€/kg 209	€ 10.8	€/kg >192	€ 14.6	€/kg 802

*Costs related to replacing articles are not calculated.

** The costs to users, alternatively the administrative costs related to derogations, are not included in these calculations.

***Reductions in Hg emissions outside EU are not included in these calculations.

F.2.9 Socio-economic benefits of the restriction

F.2.9.1 Human health impacts

The reason for a Community-wide restriction on these substances relates as much to their potential to degrade and lead to release of mercury itself to the environment, as to exposure to humans, including exposure via the environment, in particular from methylmercury.

In the context of human health impacts that would be avoided by restricting the use of these substances and thus reducing releases, it is worth noting:

- Upon releases the phenylmercury substances are degraded to metallic mercury and/or inorganic mercury, which may be transformed to methylmercury in the environment.
- Methylmercury is highly toxic, in particular to the nervous system,
- In particular the developing central nervous system is shown to be sensitive to methylmercury. Methylmercury in seafood consumed by pregnant women, even at mercury concentrations of 10-20% of those giving effects in adults, appears to have subtle, persistent effects on children's mental development
- The levels of methylmercury in fish in Europe, and in particular the data indicating increasing levels in the last 10 years in some areas, is of serious concern for human health
- The risk characterization for consumers indicates that phenylmercury acetate release from articles in the indoor environment may cause adverse health effects to consumers.

Releases of mercury from the phenylmercury compounds will contribute to health impacts such as those mentioned above (particularly transformation in the environment to methylmercury, with associated implications for health). Therefore, by reducing – and eventually eliminating – releases of mercury from these compounds, it is expected that there should be a corresponding benefit to human health.

There is considerably less data on the toxicological properties of the most suitable alternative catalysts than there is for mercury and the phenylmercury compounds. However, based on the analysis of alternatives (Part C), the alternatives are expected to pose significantly lower

health risks than those of mercury. The proposed restriction would, therefore, be expected to result in a net benefit in terms of human health impacts.

F.2.9.2 Environmental impacts

In the context of environmental impacts that would be avoided by restricting the use of these substances and thus reducing releases, it is worth noting:

- Upon releases the phenylmercury substances are degraded to metallic mercury and/or inorganic mercury, which may be transformed to methylmercury in the environment.
- Methylmercury is a PBT-like substance, the exposures and emissions to humans and the environment should be minimized to the extent possible. Consequently, releases of substances that are transformed to substances with PBT-properties should be minimized to the extent possible.
- Mercury and its compounds are highly toxic to ecosystems and wildlife, in particular there is a potential for secondary poisoning through the food chain.
- Additional releases of mercury from anthropogenic sources have led to significant increases in environmental exposure and deposition. Past releases have also created a "global pool" of mercury in the environment, part of which is continuously mobilized, deposited and re-mobilized. Further emissions add to this global pool circulating between air, water, sediments, soil and biota
- Mercury pollution is a transboundary and global pollutant. Mercury can undergo long-range atmospheric transport, which has also led to contamination of regions with few or no mercury sources, like the Arctic.

F.2.9.3 Valuation of benefits

In practice, it is not feasible – based on currently available approaches for assessment of the impacts of reducing emissions of mercury – to quantify the reduction in adverse health or environmental effects per se (i.e. damage avoided) that would be achieved through restricting the use of these compounds.

Based on the arguments above, however, an estimation of the annual emissions of mercury that is avoided by the restriction proposal is considered to be a useful indicator of the environmental (and indirectly human) impacts.

As with human health impacts, it is not considered feasible to quantify the reduction in environmental impacts associated with reducing emissions of the phenylmercury compounds and the consequent changes in environmental mercury contributions.

However, given that the analysis of alternatives concluded that the alternatives are expected to pose significantly lower environmental risks than those of mercury, it is considered likely that the proposed restriction would result in a net benefit in terms of environmental impacts.

A number of studies that try to estimate the benefits of reducing emissions of mercury have been published. In the restriction dossier on mercury in measuring devices (ECHA 2010, Appendix 2) a survey of different valuation studies is presented. None of these studies on health benefits of reducing mercury emissions are fully transferable to emission reductions from the 5 phenylmercury compounds in this document, as we have not been able to establish the level of exposure. Nevertheless, in the restriction dossier on mercury in measuring devices

the dossier submitter concludes that the majority of the studies reviewed have a benefit estimate between € 5 000 – 20 000 per kg Hg reduced.

F.2.10 Proportionality as regards costs/benefits of the restriction

F.2.10.1 Restriction on placing on the market and use

On the basis of the available information it seems clear that a restriction on the 5 phenylmercury compounds will give significant reductions in mercury emissions. As described in the respective sections above the health and environmental benefits of reducing mercury emissions are significant and are expected to outweigh the costs. The main (net) cost impact on industry arises through the replacement of mercury containing PU systems by mercury free systems and further R&D costs for those systems that are more difficult to be replaced. No social or any wider economic impacts will occur due to the restriction (see sections F.3 to F.5). Besides cost calculations (section F.2.7) a number of studies try to estimate the benefits of reducing mercury emissions. In the restriction dossier on mercury in measuring devices (ECHA 2010, appendix 2) a survey of different valuation studies is presented. None of these studies on health benefits of reducing mercury emissions are fully transferable to emission reductions from the five phenylmercury compounds. Nevertheless, in the restriction dossier on mercury in measuring devices the dossier submitter concluded that the majority of the studies reviewed have a benefit estimate between € 5000 – 20 000 per kg mercury reduced. So, despite many uncertainties and caution related to the assumptions made for the costs and benefits calculations there is a strong indication that the health benefits outweigh the estimated costs of € 2.4 million for option 1 (considered to be the best risk management option) of restricting the placing on the market and use of the five phenylmercury compounds (see Table F.7).

F.2.10.2 Restriction on manufacture

Manufacture seems to have only a minor contribution to the total emissions. Therefore the cost-benefit ratio of restricting manufacture is not as straightforward as restricting placing on the market and use. The cost-benefit ratio of restricting manufacture is mainly dependent on two factors: the behaviour of the non-EU market i.e. to what extent actors outside the EU will switch to mercury-free alternatives (or to what extent they will purchase the phenylmercury compounds from other sources than EU suppliers) and from the amount of emissions (from exports) coming back to the EU (due to the long-range transport properties of the substances). As stated above, if the non-EU market keeps on using mercury-containing catalysts produced outside the EU, there will be no (health) benefit in restricting manufacture (see section F.2.8). On the contrary, if the non-EU market totally switches to mercury-free catalysts there will be a potentially high (health) benefit in restricting manufacture. The most likely scenario will be somewhere between these two scenarios but the actual rate of substitution is unknown and a highly uncertain factor. Another highly uncertain input factor is the amount of emissions that might come back to the EU due to the long-range transport properties of mercury. In order to get an idea of the cost-benefit ratios of different possible scenarios a break-even calculation was performed. The objective was to identify the percentage of non-EU users that would have to switch to mercury-free alternatives in order for the restriction on manufacture to be cost neutral (i.e. costs equal benefits) given that it is expected that 5 % of emissions (from exports) will come back to the EU. The following input factors have been used:

Use of phenyl neodecanoate in the EU: 36 – 70 tonnes in 2008 (see Table B-1)

- Phenylmercury exports: 2.6 – 2.9 times higher than phenyl neodecanoate use in the EU, i.e. 94 – 194 tonnes in 2008 (see Table B-1). For the break-even calculations the high value (as recommended by RAC), i.e. 2.9, has been used
- Exponential decline in use and exports as stated by industry: a rate of – 9.2 % /year has been assumed (see also section B.2.3)
- Emissions from use (in EU) and exports (outside the EU): 6.38 tonnes / year of mercury emissions (see Table B-59)
- Costs based on estimations of loss of export revenue (as the cost of restricting manufacture): € 7.3 million (see Table F.7); this cost estimation is a high estimate and may in addition be overestimated due to the fact that industry indicated that production for an export market only would not continue in case placing on the market and use will be restricted
- Unit benefits values of mercury emissions avoided: in addition to the low value of € 5,000 and the high value of € 20,000 also the mid-term value of € 12,500/kg mercury avoided has been used (see section F.2.9.3); these values might still be underestimated
- Time period for cost and benefit calculations: 2018 (entry into force of the restriction) to 2028 (as considered by the dossier submitter)
- Costs and benefits calculated in 2010 NPV (net present value)
- 5 % of mercury emissions (from exports) is expected to come back to the EU (LRT properties)

On the basis of the input factors described above, the analysis considered what percentage of non-EU users would have to substitute to mercury-free alternatives in order that costs equal benefits. The outcome strongly depends on the choice of the substitution rate, the unit benefits values for mercury emissions avoided as well as the amount of emissions coming back to the EU:

Table F-8 Break-even analysis of restricting manufacture

Break-even Analysis	Unit Benefits values		
	Low = €5,000	Med = €12,500	High = €20,000
Substitution Rate	83.3%	33.3%	20.9%

As shown in the table above assuming a 5 % LRT rate, 83.3 % of the non-EU market would have to switch to mercury-free alternatives in order to make the restriction on manufacture cost neutral. This seems to be a fairly high amount but it has to be kept in mind that it is based on high values for the estimation of costs and the lowest values for the estimations of unit benefits values. When choosing the mid to high value for unit benefits values estimations (which still might be an underestimation) the necessary substitution rate ranges between 33.3 % and 20.9 %. These substitution rates might still be an overestimation: costs are calculated based on loss of export revenues but industry indicated that production for export only will be ceased anyway. So, it might be that costs are fairly lower. Moreover, the total cost of € 7.3 million seems to be low at all. Benefits could potentially be fairly underestimated, especially if global impacts, occupational health and environmental benefits were also taken into account. Input factors, particularly the substitution rate and the amount of emissions coming

back to the EU, are highly uncertain and it is not possible to conclude on their "actual" value. Nevertheless, based on the calculations undertaken, it seems that costs are not disproportionate to the benefits.

F.3 Social impacts

F.3.1 Potential for loss of employment

The main social impacts might occur related to changes in employment. Manufacturers that predominately export these mercury compounds could lose their non-EU market since non-EU manufacturers could still provide these mercury compounds. It is therefore possible there could be some net unemployment within the EU. For those manufacturers and users of mercury compounds within the EU, it is possible that any loss of employment (and production) might be offset by increases in employment (and production) by manufacturers and users of mercury-free compounds.

F.3.2 Changes in price for end users

The operating costs of using alternative mercury-free compounds are expected to be similar to using these phenylmercury substances, and virtually the same equipment is used. Since the costs of compliance (R&D) are estimated to be small, there is not expected to be any significant change to consumer prices for these products given that over 95% of the mark*et al*ready use mercury-free compounds.

F.4 Wider economic impacts

F.4.1 Minimal changes in competition

Given that the market is heavily dominated already by mercury-free catalysts, there is not expected to be a significant macro-economic impact from the restriction. The restriction will give a competitive advantage to companies producing and using mercury-free catalysts and may simply redistribute sales to existing mercury-free catalyst manufacturers and products.

The restriction may also give a "first mover" advantage to those that develop and market mercury-free alternatives for certain uses that may currently not be technically feasible or suitable.

There is not expected to be any competitiveness impacts with competitors outside of the EU as the restriction includes the restriction of imported phenylmercury substances as well as articles containing phenylmercury substances.

F.4.2 Investment and trade flows

There is likely to be some changes in both trade and investment flows since exports of these mercury compounds will be prohibited as well as imports of articles containing mercury catalysts. Export and import volumes of the compounds themselves are fairly insignificant from an EU trade volume perspective. However, the impacts on imported articles may be more significant although there is insufficient information to quantify this. Since the market is already heavily dominated by mercury-free catalysts, it is however unlikely there might be a significant detrimental impact on investment flows. In fact, there might be an increase in

investment and trade flows over time for mercury-free EU producers and products if there is a global effort to remove these mercury compounds.

F.5 Distributional impacts

As discussed above, since the market is heavily dominated already by mercury-free catalysts, the overall EU impact will not be significant. There will potentially be distributional effects with manufacturers and users of these mercury compounds seeing a premature end to their sales and associated revenue. This could also lead to loss of employment. However this might be offset by increases in employment and sales revenue for manufacturers and users of mercury-free compounds. Those that will be particularly affected will be manufacturers who predominately export the mercury compound outside of the EU.

F.5.1 Impact on SMEs

Amongst the end-users of the polyurethane systems there are understood to be many companies, some of which will be SMEs. Assuming that replacement of the phenylmercury compounds is technically and economically feasible (see above) within the timescale of the proposed restriction, the restriction should be manageable for the downstream users. We therefore do not expect there to be any impacts of importance for the SMEs.

F.6 Conclusion

Due to limited information, especially on the issue of imported articles, it has only been possible to perform a partial SEA.

However, on the basis of the available information it seems clear that a restriction on the 5 phenylmercury compounds will give significant reductions in mercury emissions. As described above the health and environmental benefits of reducing mercury emissions are significant. It has not been possible to quantify and monetize the exact benefits of reduced emissions of the 5 phenylmercury compounds subject to the restriction. However a survey of different studies performed in the restriction dossier for mercury in measuring devices (ECHA 2010, Appendix 2) indicates a benefit estimate between € 5 000 – 20 000 per kg Hg reduced. These estimates have been considered further in order to decide on the proportionality of the restriction proposal, especially as far as the inclusion of manufacture in the scope of the restriction is concerned.

It is expected that all use of mercury-containing catalysts can be replaced within a transition period of 5 years. A shorter transition period will lead to increased costs due to reduced quality of products. Alternatively derogations might be given leading to increased administrative costs. The main cost of restricting the use of these substances will be the cost of finding and developing suitable alternatives. The cost-effectiveness of the proposed restriction is estimated to be 649 €/kg. The cost of restricting manufacture is equal to the loss of value added from export. The cost-effectiveness of a restriction that does not restrict manufacture is estimated to be 159 €/kg. By restricting manufacture there may be significant reductions in emissions outside the EU, but these effects are highly uncertain.
There are no benefit estimates which are fully transferable to the emission reductions estimated. However, the lowest estimate of the benefits presented above outweighs the estimated costs of the restriction by a large margin as far as a restriction on placing on the market and use is concerned. The cost-benefit ratio of restricting manufacture is mainly

dependent on two factors, i.e. the behaviour of actors outside the EU (substitution of phenylmercury-containing catalysts by mercury-free catalysts) as well as the amount of mercury emissions (from exports) likely to come back to the EU (due to the LRT properties of the substances). These factors are highly uncertain but calculations show that the costs are not disproportionate to the benefits (see part F). Bearing all the uncertainties in mind we believe that this merit the conclusion that the benefits of the restriction proposed can be expected to outweigh the costs.

Because there is no benefit estimates which are fully transferable to the emission reductions estimated, the net benefit of the restriction has not been calculated. However, the lowest estimate of the benefits presented above, outweighs the estimated costs of the restriction by a large margin. Bearing all the uncertainties in mind we believe that this merit the conclusion that the benefits of the restriction proposed can be expected to outweigh the costs.

Many other organomercury compounds can be used as catalysts in polyurethane production. The actual use within the EU is most probably limited to a small number, see Section C.1.1.7. The 5 substances that have been included in this restriction proposal are those that have been used and manufactured in EU in significant amounts. Use of other organomercury catalysts, now or in the future, cannot be excluded. However, restricting the use of all mercury compounds as catalysts would most probably not incur any additional costs of significance. As mentioned above, no information is available on the use of any mercury compounds in imported articles.

F.7 Summary of main assumptions

A number of assumptions have been made in the analysis, in both qualitative and quantitative terms. The present report draws significantly upon data derived from the work of other organisations and there are inherent assumptions included within these analyses. Some of the key assumptions in reaching the conclusions above include:

- Data on manufacture and use of the phenylmercury compounds is confidential, in terms of the numbers of companies involved in production of the compounds and the catalysts as well as in terms of the quantities involved. It has been assumed that use of the substances (particularly phenylmercury neodecanoate) is at the upper end of the range that has been quoted to preserve the confidentiality of data. This is consistent with the approach adopted for estimation of releases to the environment.
- Potential reductions in releases to the environment associated with the restriction options are based on the assumption that releases will be proportional to the use. In this analysis the baseline scenario is assumed to be declining exponentially. This is based on the assumed historical decline and assuming a continuation of the current trend. It is assumed that use 10 years ago was 2-3 times higher than it is today. It is recognized that this assumption in itself is likely to be subject to considerable uncertainty.
- It is assumed that the number of systems still using mercury catalysts under the baseline scenario reduce at a rate equivalent to assumed reductions in mercury consumption (tonnes). Under the baseline scenario, there is assumed to be a decline in the use of mercury and there is an equivalent rate of decline in the number of systems still using mercury catalysts. It is also assumed that any reductions in systems relative to those uses will occur for those products where it is “relatively easy” to substitute with an alternative.

- A key assumption (Cowi and Concorde East/West, 2008 and Section C.5) is that the sectors concerned would be able to introduce alternatives for effectively all of the current uses of the phenylmercury compounds within 3-5 years (and 70% within 2-3 years). This is based on information from the industry and has been verified through a second consultation.
- In the calculation of cost and avoided emissions for the two restriction options we made the following assumption, in line with the point above: For restriction option 2 we are assuming that it would only be possible to replace 70 % of the systems before 2018. This means that the remaining 30 % of the systems deemed to be difficult to replace will not be substituted until 2018. The cost of replacing these 40 systems in 2018 is assumed to be the same for options 1 and 2. Subsequently only 70 % of the assumed emissions from the expected use between 2015 and 2018 are assumed avoided (for restriction option 2)
- It is further assumed that the economic lifetime of the R & D investment made to develop alternative catalysts is 10 years. The 10 years chosen is an assumption on how long the average alternative catalysts developed will be marketed. This is a considerably shorter marketing lifetime than the existing Hg-containing catalysts. The reason for choosing a shorter life span is the perception of a more dynamic market with greater competition between different catalysts and different PU systems.

The types of costs that would be incurred and the levels at which these would occur in the event of a restriction are based on information from studies already undertaken (particularly Cowi and Concorde East/West, 2008) and confirmed by the consultation undertaken for the socioeconomic assessment. In the calculations in the SEA we use the high cost estimates only, to reduce the risk of underestimating the costs.

F.8 Uncertainties

There is uncertainty related to a number of different topics in this analysis. The most important are:

- There is uncertainty with respect to the baseline, in terms of how manufacture and use of the substances will change in the future if no restriction is introduced. In this analysis the baseline scenario is based on an exponential decline based on an assumed historical decline. It is assumed that such decline is likely based on information from other studies (e.g. Cowi and Concorde East/West, 2008) that suggests that activity is ongoing to further replace these substances.
- There is uncertainty related to the number of MCPUE systems that will be difficult to substitute after the transition period. It is believed that 70% of these systems could be replaced with mercury free systems within 2-3 years, whilst the remaining 30% would be more difficult and may require additional time (3-5 years).
- There is uncertainty related to the calculated costs. The unit costs used are estimates based on available information, which has been limited. There are also uncertainties related to the future trend of the export market and therefore uncertainties related to the cost of lost export.
- There is uncertainty related to which MCPUE systems are most difficult to replace and the additional costs a premature replacement of these would entail. For example potential costs related to reduced quality of products due to inferior alternatives to Hg-containing PU-systems in the period from 2015 to 2018 if option 2 is chosen.

- Very limited information on import of articles containing phenylmercury substances is available. As a result of this import of articles is not included in the estimated emissions or in the calculated costs.
- It has not been possible to quantify the specific reduction in damages to human health or the environment that will result from this restriction. As a result of this it has not been possible to calculate the direct benefits of this restriction proposal. Instead, we have referred to studies that give us an indication that the benefits outweigh the estimated costs of the restriction (see chapter C).
- Break-even calculations on the proportionality of restricting manufacture are based on highly uncertain input factors: the substitution rate to mercury-free alternatives outside the EU and the emission factors of mercury emissions coming back to the EU (due to LRT properties)

G STAKEHOLDER CONSULTATION

Information on the phenylmercury substances and the use as catalysts in polyurethane systems has been collected on several occasions by:

- Cowi and Concorde (2008), published by DG ENV: Options for reducing mercury use in products and application, and the fate of mercury already circulating in society
- Cowi for The Norwegian Climate and Pollution Agency (this study) when assessing the manufacture and use of the substances, and when assessing the alternatives to the phenylmercury substances (two consultations, 2009, 2010)
- Entec UK Ltd for The Norwegian Climate and Pollution Agency (this study) when assessing the socio-economic costs of a restriction of the phenylmercury substances (20010)

The following have been consulted:

- EU based manufacturers of the phenylmercury compounds
- EU based formulators of phenylmercury catalysts
- EU based suppliers of chemicals or PhHg catalysts
- EU based suppliers of alternative catalysts
- EU based producers of polyurethane based articles containing phenylmercury compounds
- Trade associations

In Europe a limited number of actors are dealing with manufacture of the substances and production of catalysts, the identity of some of the companies is omitted in this report due to confidentiality.

The results of the consultations are reflected in Section B.2, B.9, C and F. Data and information are gathered for the assessment of uses and releases (Section B.2, B.9) and assessment of alternatives (Part C). A key feature of the socio-economic assessment has been consultation with the supply chain for phenylmercury products in order to understand the impact of the proposed restriction on different actors within the supply chain (Part F). In addition data are available from the report "Options for reducing mercury use in products and applications, and the fate of mercury already circulating in society" (Cowi and Concorde East/West, 2008). An overview of the number of enterprises consulted and percentage of respondents are presented in Table G.1.

Table G-1 Respondents

Category	Total number of identified enterprises using PhHg	Number of enterprises contacted	Percentage contacted of total no of identified enterprises	Number of enterprises responded	Percentage responded of total no of identified enterprises
Manufacturers of PhHg compounds	<4	<4	100	<4	100
Formulators of PhHg catalysts	<4	<4	100	<4	100
Suppliers of chemicals or PhHg catalysts (e.g formulators of 2 component systems)	~150	10	<10	6	<5
Suppliers of alternative catalysts	n.a.	6	n.a.	5	n.a.
Producers of PU based articles containing PhHg	>2200	12	< 1	10	<0.5
Trade organisations	n.a	4	n.a.	1	n.a.

In particular, the aim of the consultation for the socio-economic assessment was to gather new information and verify information on the following:

- Historic and likely future use of the phenylmercury compounds
- Potential for replacing the phenylmercury compounds in polyurethane systems
  - Costs of replacement (substitution) of phenylmercury compounds
  - Main barriers to substitution (technical and/or financial)
- Specific uses for polyurethane systems containing phenylmercury
- Impact of the restriction on actors within the supply chain
  - Export market for phenylmercury products
  - manufacture and use of phenylmercury catalysts
  - manufacture and use of PU systems that use mercury catalysts

Consultation for studies such as this can be difficult as it is not always possible to find the correct contacts or to elicit the information required (for example to find exact and specific uses for PU products), as much of it is commercially confidential or not available. Nevertheless, a considerable amount of useful information was gathered to inform this study. A summary of that information (made anonymous for the purpose of this report), is presented in Table G-2.

Table G-2 Summary of consultations for the socio-economic assessment

Supply chain sector (based in EU)	Summary of findings	Use in study
Manufacturers of phenylmercury substances	Confirmation that phenylmercury acetate and 2-ethylhexanoate are all exported outside of the EU. EU market for phenylmercury compounds is dependent on the export market and vice versa. This is because the price paid for raw material (i.e. mercury) is dependent on the volume bought. Also there are fixed costs for processing the products including costs for environmental controls that are not volume dependent. It would therefore not be viable to have export market alone. It is understood that mercury products are high value and support the production of other non mercury products (if also produced). Up to 70% of sales value of products due to sales of mercury based products. It would take 6 or 7 years to establish a market for other (non-mercury) products. It is likely that production of phenylmercury products would not continue beyond 2013.	Confirmation of import export of products. Understanding of market for products (declining globally). Understanding of affect of restriction on manufacturers. Understanding of impact of restriction with/without manufacturing (i.e. with/without) export market.
Formulators of phenylmercury catalysts	Market appears to have been stable for particular products use for PU systems for a number of years. Indicated that a restriction would not cause great impacts as products are a relatively small part of their product portfolio	Informing the baseline scenario for phenylmercury products.
Formulators of PU systems using phenylmercury catalysts	Use of catalyst products is based only on neodecanoate. The use in products mentioned below has been stable over recent years. Mercury based catalysts are used for 5-6 products, including repair of rubber components and sealants. The products for repair are particularly important for use in the oil and gas offshore applications for repair of different types of components, (e.g. parts of instruments that could wear with time or long lasting installations and extreme environments). High price for products indicated (>€800/kg).	Understanding of the impacts of the proposed restriction. Costs of products and replacement (substitution) of products.

Supply chain sector (based in EU)	Summary of findings	Use in study
	Alternatives are not suitable because of lack of strength and durability of final products. It is not expected that all uses would be covered by alternatives within 5 years without legislative action. Mercury catalysts are selected for a number of uses because of properties which alternatives do not provide. The main costs incurred would be the R&D to find suitable alternative systems for customers – the costs are passed on in the prices of the systems sold. It appears that no changes in equipment are necessary for the development t of system using alternatives. Restriction would lead to loss of sales.	
Users of PU systems with phenylmercury catalysts	No positive responses from those consulted; apart from responses to inform that mercury based catalysts are no-longer used.	
Users of formed PU product containing phenylmercury catalysts	Unable to identify without precise and specific knowledge of the articles being used.	
Suppliers of alternative catalysts	Unable to get specific information on uses	
Trade associations	Trade association contacted ISOPA (Manufacturers of substances used to make PU systems (polyols and isocyanates)). Although used for niche applications, the issue of the restriction of phenylmercury substances was not considered to be an important issue for the members of this trade organisation.	Relative importance of this to large producers substance used to make PU plastics in the global market.
Consultation with consultants for other reports	Calculations on costs for substitution were based on consultation with two people from same company providing PU systems to users. Cost estimates were based on actual estimation of R and D time and opportunity costs (i.e. the time spent on other tasks if R and D did not have to be done). Additional costs were based on less personal experience - i.e. "opportunity cost might add only 10-20% to the €3.5-5.0 million calculated above. If the phase-out were required over 2-3 years, the opportunity cost might add as much as 40-50%." from report is based more on a estimate between the consultant and interviewees.	Reliability of cost information on substitution quoted in Cowi and Concorde East West (2008).

H H OTHER INFORMATION

No additional information included.

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Appendix 1: Quantitative health and environmental risk characterisation, including derivation of PEC and PNEC values for the aquatic and terrestrial compartment

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1. Predicted environmental concentrations (PEC)

Environmental concentrations at regional level have been calculated by the EUSES version 2.1.1 software, using the default regional environmental parameters (TGD, Part II, table 12 p. 88), Appendix 6. It was not considered feasible to calculate local concentrations based on the information available. It has to be emphasized that the EUSES model does not account for degradation of toxic chemicals to equally or more toxic degradation products, which is the case for phenylmercury compounds. We are aware of the fact that the estimated environmental concentrations of mercury in the different compartments are considerably affected by the physical chemical properties of the mercury species used for the modeling. Phenylmercury compounds are degraded to metallic or ionic mercury with diphenylmercury as an intermediate degradation product. Inorganic mercury is part of the biogeochemical mercury cycle with ionic, metallic and methylmercury as main species. As the EUSES model uses the physical chemical properties of only one single mercury species, the model cannot estimate an appropriate distribution of phenylmercury compounds and their degradation products in the environment. Therefore, the predicted environmental concentrations (PECs) should be understood as rough estimates.

The calculations have been performed using the substance properties of phenylmercury acetate (which is the only of the compounds for which sufficient data are available), however, assuming that the substance is not biodegradable as elemental mercury was identified as the relevant component for risk assessment. The release estimation was based on the total consumption volume of all fiveour compounds in terms of elemental mercury, i.e. 31.33 tonnes/year, and the distribution of releases to the environment was conducted as summarised in Section B.9.6.1.

As there are numerous specific uses of PU elastomers and many companies are involved in the production as formulators and/or end-users EU-wide, the use category selected was "55/Others" while "multi-purpose equipment" was selected as main production category. The input parameters used for the EUSES modeling are listed in Appendix 6.

1.1 Regional concentrations

Atmosphere

Regional PEC, atmosphere: 3.42E-8 µg/m3
Continental PEC, atmosphere: 1.96-8 µg/m3

Aquatic compartment

Regional PEC, surface water (total): 2.78E-03 µg/L
Continental PEC, surface water (total): 2.36E-03 µg/L

Regional PEC, sea water (total) 3.06E-04 µg/l
Continental PEC, sea water (total) 3.92E-05 µg/l

Sediment

Regional PEC, sediment: 0.93 µg/kg wwt
Continental PEC, sediment: 0.79 µg/kg wwt

Regional PEC, seawater sediment 9.27E-02 µg/kg wwt
Continental PEC, seawater sediment 1.19E-02 µg/kg wwt

Soil compartment
Regional PEC, soil: 0.63 µg/kg wwt
Continental PEC, soil: 0.36 µg/kg wwt

1.2 Local concentrations
Not calculated.

2. Predicted no effect concentrations (PNEC)

2.1 PNEC determination for the aquatic environment including sediment

Phenylmercury compounds are degraded in the environment to hazardous degradation products as i.e elemental mercury and divalent mercury, which can be transformed to methylmercury. The inorganic mercury species are expected to be the dominant species of mercury in the environment. The quantitative risk characterization is therefore based on the hazardous degradation products, and the PNECs for the aquatic and terrestrial compartment are based on PNEC for divalent mercury. However, for the sake of completeness the PNEC for phenylmercury acetate (PMA) is presented. No PNEC for methylmercury was estimated because for this PBT-like compound a qualitative risk is sufficient and would override the quantitative risk assessment.

2.1.1 PNEC aquatic

Phenylmercury acetate

Summary of effects
Data selected on the most relevant endpoints for both acute and chronic toxicity to phenyl mercury acetate:

	Species	Value	Remarks/Justification
Acute toxicity	Mosquito fish (Gambusia affinis)	37 µg/L	96 h LC50 (Joshi and Rege ,1980)
	Zebrafish (Danio rerio)	30 µg/L	LOEC Non hatching of eggs (Kihlström and Hulth, 1972)
	Rainbow trout fingerlings (Onchorynchus mykiss)	8.6 µg/L	96 h LC50 (Matida et al., 1971)
	Intertidal crab (marine) (Scylla serrata)	540 µg/L	96 h LC50 (Krishnaja et al., 1987)
	Algae (Chlamydomonas variabilis)	>1 µg/L	Growth affected by a lag phase before the exponential growth phase (Delcourt and Mestre, 1978)
	Brown mussel (marine)	20 µg/L	50% reduction in filtering rate (Watling and Watling, 1982)

	(Perna perna)		
Chronic toxicity	Rainbow trout (Onchorynchus mykiss)	1.1/0.11 µg/L	12 weeks LOEC/NOEC on growth (Matida et al., 1971)
	Intertidal crab (marine) (Scylla serrata)	<180 µg/L	30 days NOEC (Krishnaja et al., 1987)
	Water flea (Daphnia magna)	1.90/1.12 Hg µg/L	21 days LOEC/NOEC survival (Biesinger et al., 1982)

Phenylmercury propionate, -octanoate, 2-ethylhexanoate and -neodecanoate
No data found.

PNEC-derivation
Acute and chronic toxicity data to PMA have been assessed for the PNEC derivation. The Daphnia magna chronic study by Biesinger et al. (1982) is considered to be the most robust dataset. A NOEC of 1.12 µg/L for survival after 21 days exposure has been selected for the derivation of the PNEC. The assessment factor chosen is based on two NOEC values of two different trophic levels as detailed in the Reach guidance.
With regards to the PNEC for the marine environment, an assessment factor of 500 has been used as there are only two long term results (NOEC) for freshwater/saltwater available representing two trophic levels fish (rainbow trout) and crustacean (Daphnia magna). Further effect data on additional marine taxonomic groups are not available.

	Value	Assessment factor	Remarks/Justification
PNEC freshwater	0.0224 Hg µg/L	50	Based on the study by Biesinger et al., (1982)
PNEC marine	0.0022 Hg µg/L	500	Based on the study by Biesinger et al., (1982)

Phenylmercury propionate, -octanoate, 2-ethylhexanoate and -neodecanoate
No PNEC was derived due to the lack of toxicity data.

Inorganic mercury
For mercury compounds that are part of the biogeochemical mercury cycle (see Section B.4.1.3), PNEC's were developed in the scope of the Water Framework Directive (WFD). Background information on the setting of environmental quality standards have been compiled and evaluated in a supporting background substance data sheet for mercury and its compounds EC (2005).

In this document the maximum permissible addition is equated with the PNEC. The maximum permissible addition is the amount of metal that maximally may be added to the naturally occurring background concentration of this metal without adversely affecting the assessed ecosystem. For further details on that approach see also the manual of methodological framework used to derive environmental quality standards for priority substances of the water framework directive (2004).

Freshwater
There are many long-term no effect and short-term acute toxicity data for a broad range of species from different taxonomic groups available. With regard to long-term/chronic exposure, algae, fish and crustaceans appear to be the most sensitive groups in freshwater whereas in saltwater molluscs and coelenterata (e.g. jellyfish) appear to be even more sensitive than the before mentioned groups. The lowest NOEC has been obtained for the marine coelenterate Clavopsella michaeli (0.1 µg/l) but the lowest freshwater toxicity test result is only slightly higher (0.2 µg/l, EC10 of Scenedesmus acuminatus). The appropriate assessment factor according to the Technical Guidance Document (TGD,2003) is 10 (long-term toxicity data across at least 3 trophic levels for 3 different taxonomic groups are available and the species for which the lowest acute result has been obtained belongs to the groups for which long-term data are available). Therefore the PNEC is calculated as follows:

PNECfreshwater = 0.1 µg/l / AF (10) = 0.01 µg inorganic mercury /l

Saltwater
As there is obviously no difference in the lower limit of the sensitivity range of freshwater and saltwater species (se statistical extrapolation below), it is suggested to derive the PNEC applicable to freshwater or saltwater environments from the same data set.
A comprehensive data base on marine species is available and it is suggested in accordance with the REACH guidance to apply a safety factor of 10 on the lowest reported NOEC. Hence, the suggested PNEC for the saltwater pelagic community is equal to that calculated for freshwater.

PNECsaltwater = PNECfreshwater = 0.01 µg inorganic mercury /l,

Calculation of the maximum permissible addition by statistical extrapolation

For metals with large databases (including many long term toxicity data of a range of aquatic species) it is proposed to use a statistical extrapolation method as standard method for the calculation of the maximum permissible addition. The method of Aldenberg and Jaworska (2000) seems suitable for this purpose as it is possible to calculate a confidence interval (normally the 90% interval) for the 5-percentile cut-off value of the species sensitivity distribution (SSD). The 5-percentil cut-off identifies the concentration that protects 95% of the biological species that are included in the calculation.
For mercury longterm/ chronic NOECs are available for 9 different taxonomic groups (freshwater & saltwater together, 7 groups for each of the environments). Tests with higher plant species are missing but it is known that higher plants are not particularly sensitive to mercury. The detailed description of the application and results of the statistical extrapolation method are described in the background substance sheet mercury and its compounds EC (2005). The 5-percentile cut-off value (5P-COV) of the species sensitivity distribution have been calculated with 3 data sets.

Table 2.1.1: Results of the sensitivity distribution method:

		90 % Confidence Interval	
Data set	5-Percentile Cut-Off Value (50% confidence)	5P-COV (95% conf.)	5P-COV (5% conf.)
1. Combined NOECs	**0.142**	**0.054**	**0.284**
2. Freshwater NOECs	0.160	0.022	0.332
3. Saltwater NOECs	0.143	0.033	0.360

From the data given in Table 2.1.1 it can be seen that the 50% confidence 5P-COVs for the freshwater and saltwater data sets are nearly identical. It is therefore deemed appropriate to use the 5P-COV of the combined freshwater and saltwater NOECs for the calculation of the maximum permissible addition. In order to derive the PNEC, which is equated with the maximum permissible addition, it is suggested in the TGD to divide the 5P-COV by an appropriate assessment factor between 1 and 5, reflecting further uncertainties identified. An assessment factor of 3 has been used for the derivation of the PNEC. The details on the selection of the appropriate assessment factor are described in the background substance sheet mercury and its compounds (EC 2005).

PNECwater.SSD = 5P-COV (0.142 µg/l) / AF (3) = 0.047 µg inorganic mercury /l

As the PNEC based on statistical extrapolation is with more than 95% confidence lower than the concentration that probably could affect 5% of the species it is suggested to use this value for the risk characterization.

2.1.2 PNEC sediment

Phenylmercury acetate
No effect data of PMA on sediment dwelling organisms are available. Since phenylmercury compounds are degraded to hazardous degradation products the PNECsediment for inorganic mercury will be used in the risk characterisation.(EC 2005)

Phenylmercury propionate, -octanoate, 2-ethylhexanoate and -neodecanoate
No data found.

Mercury and its compounds
Since phenylmercury compounds are degraded to elemental and divalent mercury, the PNECsediment for inorganic mercury is presented and will be used in the risk characterisation. For more details on the derivation, we refer to the background substance sheet mercury and its compounds (EC 2005). The equilibrium partitioning approach is used and it only considers uptake via the water phase. However, uptake may also occur via other exposure pathways like ingestion of sediment and direct contact with sediment. In such cases it is recommended to use the equilibrium method in a modified way and apply an additional assessment factor of 10 when estimating the PNEC. For mercury there is clear evidence that exposure routes other than direct uptake via the water significantly contribute to its uptake into biota. According to the TGD the water-sediment partition coefficient is used for the calculation. The mean partition coefficient of the Rhine (Kp 100,000 l/kg) is used as an example. The PNEC sediment is calculated as follows:

PNECsediment = Kp (100,000 l/kg) * PNECwater (0.047 µg/l) / 10 = 0.47 mg inorganic mecury /kg wwt

2.2 PNEC soil

Calculation of Predicted No Effect Concentration (PNECsoil)
For phenylmercury acetate, it is not possible to calculate the PNECsoil because only a few studies were available for microorganisms. These studies were not designed to estimate EC50-values, and NOECs could not be determined. Due to the lack of toxicity data for phenylmercury proprionate, 2-ethylhexanoate, octanoate and neodecanoate, it is not possible to derive a PNEC for these substances either. The phenylmercury compounds are degraded to hazardous degradation products, i.e. divalent and elemental mercury that can be transformed to methylmercury. Risks that might arise from the degradation/transformation products of PMA have been assessed. As the percentage of methylmercury in soils normally is low, the PNECsoil is based on mercury (II), the predominant degradation product of the phenylmercury compounds in soils.

Summary of effects
Data selected on the most relevant endpoints for phenyl mercury acetate:

Method	Results	Remarks	Reference
Toxicity of divalent mercury to the enchytraeid worm Enchytraeus albidus; worms were exposed to contaminated soil	the 42-day NOEC was 18 mg Hg kg-1 soil dry weight	The test was according to OECD and ISO guidelines, but only nominal concentrations were quoted; Klimisch code 1-2	Lock and Janssen, 2001
Toxicity of divalent mercury to the earthworm Eisenia fetida exposed to contaminated soil	The 21-day NOEC was 10 mg Hg kg -1 soil dry weight	see above	Lock and Janssen, 2001
Toxicity of divalent mercury to the springtail Folsomia candida exposed to contaminated soil	The 28-day NOEC was 1.8 mg Hg kg-1 soil dry weight	see above	Lock and Janssen, 2001

Method	Results	Remarks	Reference
Soil bacteria (46 strains) were exposed to divalent mercury; mercury was present in the agar medium	The NOEC was 1 mg Hg L-1 agarsubstrate	No guidelines were used but the study is well documented; Klimisch code 2	Abou-Shanab et al., 2007
Toxicity of divalent mercury to the earthworm Octochaetus pattoni exposed to contaminated soil	60-day LD50 was 0.79 mg kg-1 soil	Methods are not sufficiently described, it is not sure if the concentrations are related to dry weight of soil; statistical analysis is missing; Klimisch code 3-4	Abbasi and Soni, 1983
Toxicity of divalent mercury to the grasshopper Aiolopus thalassinus, eggs were transferred to contaminated sand	EC100 of 0.605 mg Hg kg-1 sand dry weight; no egg hatched	No guidelines were used but the study is very well documented; Klimisch code 2	Devkota and Schmidt, 1999
Toxicity of divalent mercury to the springtail Paronychiurus kimi exposed to contaminated soil	The 28-day EC50,Reproduction was 0.23 mg kg-1 dry soil	Test was performed according to OECD and ISO guidelines but no standard species was used and only nominal test concentrations were quoted; Klimisch code 2	Son et al., 2007
Toxicity of divalent mercury to the bird rape (Brassica rapa).	A LOEC of 10 mg/kg dry soil was determined. The effect of HgCl2 on bloom initiation was measured in Hg-spiked sandy soil.	No standardized guidelines were followed but the study is well documented; Klimisch code 2	Sheppard et al., 1993

Method	Results	Remarks	Reference
Toxicity of divalent mercury to the grasshopper Aiolopus thalassinus, eggs were transferred to contaminated sand	An EC20 of approximately 0.121 mg Hg kg-1 sand dry weight. In controls 62.17% of eggs hatched at a concentration of 0.121 mg Hg kg-1 sand dry weight 50.8 could undergo embryonic development	No guidelines were used but the study is very well documented; Klimisch code 2	Devkota and Schmidt, 1999

The table shows some NOECs for soil organisms. The lowest value is not a NOEC in this case. The most sensitive endpoint is chosen for the derivation of the PNEC.

Derivation of PNECsoil

The lowest effect concentration found in literature is 0.121 mg kg-1 dry soil and is determined for the grasshopper species Aiolopus thalassinus. For divalent mercury, long term toxicity data were found for three trophic levels with a LOEC of 10 mg/kg for terrestrial plants (Sheppard et al., 1993), a NOEC of 1 mg/l for microorganisms (Abou-Shanab et al., 2007) and an EC20 of 0.121 for soil invertebrates (Devkota and Schmidt, 1999). According to the Technical Guidance Document (TGD, 2003) an assessment factor of 10 should be applied if chronic toxicity data for three trophic levels are available. However, an assessment factor of 50 is used here because the lowest value found in literature is not a NOEC but an EC20 and phenylmercury compounds are assumed to be more toxic to terrestrial organisms than Hg (II) (see Section B.7.2.1). The PNECsoil is calculated to be 2.42 µg Hg (II) kg-1 dry soil.

	Value	Assessment factor	Remarks/Justification
PNECsoil	2.42 µg Hg (II) kg-1 dry soil	50	Devkota and Schmidt, 1999

The lowest effect concentration is 0.121 mg kg-1 dry soil. According to the Technical Guidance Document (TGD, 2003) an assessment factor of 10 should be applied if NOECs for long-term toxicity tests of three species of three trophic levels are available. This is the case for Hg (II). However, an assessment factor of 50 is used because the lowest value in the table is not a NOEC but an EC20 and phenylmercury compounds are assumed to be more toxic to terrestrial organisms than Hg (II) (see Section B.7.2.1). The PNECsoil is calculated to be 2.42 µg Hg (II) kg-1 dry soil.

2.3 PNEC for sewage treatment plant

For organic mercury a NOEC of (0.2 µg/L) is obtained from the INERIS (2000) report and has been used for the derivation of the PNEC. Limited information about this study is available but according to the REACH guidance an AF of 10 has to be applied to NOEC's or EC10 of a sludge respiration test or comparable tests.

	Value	Assessment factor	Remarks/Justification
PNEC STP	0.02 µg/L organic mercury	10	

2.4 PNECsecondary poisoning

Phenylmercury acetate
Chronic dose studies are needed to assess environmental hazards. Only the study of Fitzhugh et al. (1950) provides sufficient data for a chronic, orally applied phenylmercury acetate diet in mammals.

Method	Results	Remarks	Reference
Renal damage was studied in rats fed on a chronic phenylmercury diet for up to two years	NOEC of 0.0084 mg PMA kg-1 body weight, chronic diet	The study is too old to follow a certain guideline, it is well documented but the statistical analysis is not sufficiently described and some of the graphically shown data are not sufficiently described as well; Klimisch code 2-3	Fitzhugh et al. (1950) cited in EPA, (2010)

Fitzhugh et al. (1950) studied the effects of phenylmercury acetate on rats and found a chronic NOEC of 0.1 ppm mercury per kg diet (chronic diet) for renal damage. The NOEC of 0.1 ppm was expressed as mercury equivalents and not as phenylmercury acetate. For the estimation of the PNECoral, the chronic NOEC is divided by an assessment factor of 30 according to the Technical Guidance Document (TGD, 2003). Fitzhugh et al. (1950) (EPA, 2010) assumed that rats consume the equivalent of 5% of their body weight and calculated a NOECmammal of 0.28 µg PMA kg-1 body weight.
PNECoral = 0.1 mg kg-1 · 5% · 336.74 g mol-1/(200.59 g mol-1 · 30) = 0.28 µg PMA kg-1 body weight

	Value	Assessment factor	Remarks/Justification
PNECoral for PMA (secondary poisoning)	0.28 µg PMA kg-1 body weight	30	Fitzhugh et al. (1950) cited in EPA, (2010)

Methylmercury

Summary of effects

Method	Results	Remarks	Reference

Toxicity of methylmercury to the falcon Falco sparvinus fed on a chronic diet (59 days) containing 3.2 (measured concentration) mg kg-1 dry weight	No bird died or and no signs of neurotoxicity, higher levels of mercury in whole blood, kidney , liver and breast muscle compared to untreated animals, no chick survived	The study is in part well documented but the reproductive effects remain unclear and are not sufficiently described; Klimisch code 2-3	Bennett et al., 2009
Reproductive toxicity of methylmercury to the falcon Falco sparvinus fed on a chronic diet containing 0.7 mg kg-1 dry weight	Number of fledglings and nestling fledged reduced, population decline is predicted	The study is well documented but is not according to a certain guideline; Klimisch code 2	Albers et al., 2007
Effects of a 0.5 ppm methylmercury diet on reproduction and behavior of three generations of mallard ducks Anas platyrhynchos were studied	Percentage of eggs outside nestboxes increased, fewer ducklings hatched, small amount of eggshell thinning, ducklins less responsive to tape-recorded maternal call but hyper-responsive to a frightening stimulus in avoidance tests	No guideline was used but the study is well documented, statistical design could be explained more detailed; Klimisch code 2-3	Heinz, 1979

The LOEC of the falcon study of Albers et al. (2007) is 0.7 mg kg-1 MeHg dry weight. In this experiment different doses and responses have been studied but still a chronic diet of 0.7 mg kg-1 MeHg dry weight is supposed to end in population decline (EPA, 2009). Heinz (1979) found effects in ducks fed on a diet containing 0.5 mg kg-1. This value is treated as a LOEC even though no different doses and responses were tested. The NOEC is calculated to 0.25 mg kg-1 by dividing the LOEC by a factor of 2. This NOECbird is divided by an assessment factor of 30 because effects of a chronic methylmercury diet were studied. The calculation is according to the Technical Guidance Document (TGD, 2003).
PNECoral = 250 µg kg-1/30 = 8.33 µg MeHg kg-1 diet.

	Value	Assessment factor	Remarks/Justification
PNECoral for MeHg (secondary poisoning)	8.33 µg MeHg kg-1 diet	30	Heinz, 1979

Mercury (II)
Summary of effects

Method	Results	Remarks	Reference
Reproductive toxicity of inorganic mercury in Rattus norvegicus forma domestica (Sprague-Dawley rats) was studied. The rats received 2 mg HgCl2 per kg body weight and day for 90 days	Significantly fewer implantations, more non-viable implantations, lower progesterone, higher levels of luteinizing hormone	The study does not follow any guideline but is well documented and provides suffient data; Klimisch 2	Heath et al., 2009
Reproductive toxicity of inorganic mercury in Rattus norvegicus forma domestica (Sprague-Dawley rats) was studied. The rats received 1 mg HgCl2 per kg body weight and day for 90 days	Significantly more non-viable implantations compared to controls	The study does not follow any guideline but is well documented and provides suffient data; Klimisch 2	Heath et al., 2009

Only few long-term studies were available that could be used for PNEC derivation. In general studies should be chosen that do not choose survival as the toxicological endpoint. Survival is a very rough parameter. However, if long-term and sublethal toxicity data are available, these should be preferred for risk characterisations.
Heath et al. (2009) studied the effects of a 90 day HgCl2 diet. Animals that ingested 1 mg HgCl2 per kg body weight and day showed no physical signs of Hg intoxication except from weight gain. Females had more non-viable implantations than those of controls.
It is arguable to appoint a LOEC because only two concentrations have been tested. The study provides no NOEC. If one would assume 1 mg HgCl2 per kg body weight and day as the LOEC, the NOEC is calculated to 0.5 mg HgCl2 kg-1 bw · d-1 (by dividing the LOEC by a factor of 2). The PNECoral is calculated by dividing the NOECmammal by a factor of 90. According to Technical Guidance Document (TGD, 2003) this assessment factor is used as the data were obtained in a long-term study.
PNECoral = 0.5 mg HgCl2 kg-1 bw · d-1/90 = 5.56 µg HgCl2 per kg body weight and day

	Value	Assessment factor	Remarks/Justification
PNECoral for Hg (II) (secondary poisoning)	5.56 µg HgCl2 per kg body weight and day	90	Heath et al., 2009

3. Quantitative risk characterisation

3.1 Human health

In Section B.5.11 a DNEL was derived for one of the phenylmercury compounds – PMA. Data was not available to derive DNELs for the other phenylmercury compounds. In the following this DNEL is compared with the hypothetical release from an article (swivel chair), applying the ECHA Guidance R.17 (ECHA, 2008b). A comparison of the derived DNEL for elemental mercury with release from school gymnasium flooring is also reported here.

3.1.1 Risk characterization ratios

Phenylmercury acetate

The five phenylmercury substances are used in many different products that consumers may be exposed to in everyday life. In chapter B.2.2 the use of these substances are addressed. The consumers are exposed mainly via emission from coated surfaces, sealants and filling materials and plastic articles (rollers for swivel chairs, roller skates, bumpers, wheel covers, door handles, phones, computers, skis, bicycles, hifi equipment, kitchen ware and metal office furniture, etc). It is likely that there are several articles in the indoor environment that contain and release these mercury substances at the same time. The total level that the consumers are exposed to daily is difficult to estimate. We therefore selected the release of PMA from rollers on a swivel chair, as one possible example of emission source in the indoor environment that is relevant to many people.

To our knowledge emission of PMA or other phenylmercury compunds as such from articles has not been measured. From the data in literature it cannot be concluded if PMA in the article is converted to elemental mercury prior to volatilizing, or if it is converted to elemental mercury in air (see B9). For the sake of completeness a theoretical estimation of emission and air concentrations of PMA from wheels on a swivel chair in a bedroom has been made.

During service life, articles typically contain 0.2-0.80.1-0.6% phenylmercury compounds. In the calculation we have used 0.1 and 0.6 %. The weight of 5 wheels is approximately 1500 g (pers. comm.). In this estimation it is assumed that all PMA is released as PMA and not degraded into other compounds which one would expect.

According to “Guidance on information requirements and chemical safety assessment, chapter R.17: Estimation of exposure from articles” in a screening approach it is assumed that 100% of the substance will be released during 24 hours into the room and that there is no

ventilation (ECHA, 2008b). A default value for the volume of a small bedroom is 16 m3 (Bremmer et al., 2006). Based on these exposure conditions a worst case scenario was estimated.

For articles containing 0.6 % PMA:
1500 g * 0.6 % PMA = 9 g PMA
9000 mg/ 24 h =375 mg/h
375 mg/ 16 m3 = 23.4 mg/m3

For articles containing 0.1 % PMA:
1500 g * 0.1 % PMA = 1.5 g PMA
1500 mg/ 24 h = 62.5 mg/h
62.5 mg/ 16 m3 = 3.9 mg/m3

The estimated DNEL for PMA is 0.000183 mg/m3. Using the estimated exposure scenarios, the following risk characterisation ratio (RCR) can be derived for the general population:
Instantaneous release of all the PMA taking 24 hours:
For articles containing 0.6 % PMA: RCR = Exposure/DNEL = 23.4 mg/m3/0.000183 mg/m3= 127 869
For articles containing 0.1 % PMA: RCR = Exposure/DNEL = 3.9 mg/m3/0.000183 mg/m3= 21 311

Since the RCR is much higher than 1 (up to 128 000) in these worst case scenarios a refinement of the exposure scenarios was derived. In the refinement a default value for the volume of a small bedroom is 16 m3 and a default ventilation rate is 1 h-1 (Bremmer et al., 2006). The exposure is estimated to be continuously (i.e. 24 hours a day). For the emission, it is assumed that all PMA in the article is released within 15 years. The half life t1/2 for mercury from the PU floorings has been estimated to be 16 years (ATSDR, 2008). Therefore, it is likely that the assumption of 15 years for release of all the PMA is an overestimation of the exposure compared with in real life. Exposure and corresponding RCR, when the emission time was 30 years, were also estimated.

Release of PMA taking 15 years:
For articles containing 0.6 % PMA:
1500 g * 0.6 % PMA = 9 g PMA
9 g /15 years = 0.6 g/year = 1.64 mg/d = 0.0685 mg/h
(0.0685 mg/h / 16 m3) / 1 h-1 = 0.0043 mg/m3 = 4.3 µg/m3

For articles containing 0.1 % PMA:
1500 g * 0.1 % PMA = 1.5 g PMA
1.5g /15 years = 0.1 g/year = 0.274 mg/d = 0.01142 mg/h
(0.01142 mg/h / 16 m3) / 1 h-1 = 0.00071 mg/m3 = 0.71 µg/m3

Using the estimated exposure scenarios the following risk characterisation ratio (RCR) can be derived for the general population:

Release of PMA taking 15 years:
For articles containing 0.6 % PMA: RCR = Exposure/DNEL = 4.3 µg/m3/0.183 µg/m3= 23.5
For articles containing 0.1 % PMA: RCR = Exposure/DNEL = 0.7 µg/m3/0.183 µg/m3= 3.8

Release of PMA taking 30 years:
For articles containing 0.6 % PMA:
1500 g * 0.6 % PMA = 9 g PMA
9 g /30 years = 0.3 g/year = 0.82 mg/d = 0.034 mg/h
(0.034 mg/h / 16 m3) / 1 h-1 = 0.0021 mg/m3

For articles containing 0.1 % PMA:
1500 g * 0.1 % PMA = 1.5 g PMA
1.5g /30 years = 0.05 g/year = 0.137 mg/d = 0.0057 mg/h
(0.0057 mg /h / 16 m3) / 1 h-1 = 0.00036 mg/m3

Using the estimated exposure scenarios the following risk characterisation ratio (RCR) can be derived for the general population:

Release of PMA taking 30 years:
For articles containing 0.6 % PMA: RCR = Exposure/DNEL = 2.1 µg/m3/0.183 µg/m3= 11.5
For articles containing 0.1 % PMA: RCR = Exposure/DNEL = 0.36 µg/m3/0.183 µg/m3= 2

If all the PMA is released, to the unlikely event all in 24 hours, the RCR is approximately 128 000 and 21 000 when the swivel chair contain 0.6% and 0.1% PMA, respectively. Assuming that the emission time for PMA is 15 years, the RCR is approximately 23 when the wheels contain 0.6% PMA, while if the wheels contain 0.1% PMA the RCR is approximately 4. When the emission time is extended to 30 years, the RCR is approximately 11 and 2 when the wheels on the swivel chair contain 0.6% and 0.1% PMA, respectively.

The general population may be exposed to several articles containing PMA or other phenylmercury substances simultaneously in the indoor environment. The emission rate of mercury substances from the rollers on a swivel chair is not known. Neither is the emission rate of mercury substances from most other articles containing these phenylmercury substances. The only article containing PMA, to which we know the emission rate, is the polyurethane floor. The half life for the PMA in these floors was therefore used as a proxy for the duration of emission for PMA from the rollers. However, it might be that the emission is higher due to hard use, or it might be lower due to properties of the plastic compared to the polyurethane floors.

The wheels on a swivel chair were used as an emission source in these exposure estimations. Since there might be several articles that contain these phenylmercury substances in the indoor environments, the total exposure level could be higher than indicated by the estimations based on a swivel chair. This assumption justifies the use of a 24 hours exposure time and a room size of 16 m3. Further uncertainty is due to the time-dependent emission of PMA from articles. This time-dependenc is not linear and it is likely that the articles release more mercury substances when they are new than after several years.
Following these exposure scenarios, based on the available information and the longest half-life, the risk characterisation indicate that the PMA release from articles in the indoor environment is not adequately controlled.

Phenylmercury propionate
No data.
Phenylmercuric octanoate

No data.
Phenylmercury neodecanoate
No data.
Phenylmercury 2-ethylhexanoate
No data.

Elemental mercury. Measured air concentrations from PU elastomer floorings.
For the general population a DNEL of 0.16 µg/m3 was derived based on the subtle effects on the central nervous system demonstrated in long-term occupational exposures to mercury vapour. Actual investigations of mercury release from articles have only been identified from PU elastomer flooring. PU flooring with mercury catalyst has previously been widely used in school gyms and sports arenas in the U.S.A. (and probably also in Europe). The use of phenylmercury compounds in flooring may be considered a worst case exposure scenario as the floors have large surface area from which the mercury can be released. The detectable air concentrations of mercury measured above the gymnasium floors is in the range of 130 – 2900 ng/m3 (Section B.9.3.1 Exposure of humans). Using the highest value measured as a worst case scenario the following risk characterisation ratio (RCR) can be derived for the general population:

RCR= Exposure/DNEL = 2.9/0.16 = 18.125

The RCR of 18.13 indicates that risk is not controlled.

Using the lowest measured value of 130 ng/m3 and the DNEL for the general population gives a RCR of 0.13/0.16 = 0.81, which suggests that the risk is adequately controlled. The majority of measurements from gymnasium floors reported would, however, result in a RCR>1. It should be noted that this calculation is based on a DNEL derived from a LOAEC adjusted to continuous exposure 24 hours/day, 7 days/week, see section B.5.11.

3.1.2 Exposure of man via the environment. Exposure from fish.

Mercury released to the environment from the application of phenylmercury compounds contributes to elevated levels of mercury found in the environment and thereby contributes to the exposure of humans to mercury via the environment. The phenylmercury compounds are degraded to hazardous degradation products, i.e. inorganic mercury compounds and elemental mercury, which can be transformed to methylmercury. However sufficient information for the phenylmercury compounds is not available to make a quantitative risk assessment of the possible exposure level of man via the environment.

The amounts of phenylmercury compounds released into the environment, calculated as mercury, may be compared with information on the overall emission of inorganic mercury. Inorganic mercury converted into methylmercury via anaerobic bacterial metabolism ends up in fish. Mercury is present in fish and seafood products largely as methylmercury, and fish is a useful indicator of human exposure. Food sources other than fish and seafood products may contain mercury, but mostly in the form of inorganic mercury (EFSA, 2004).

Mercury is present at low concentrations in human tissues due to background exposure from dietary intake of methylmercury from fish and shellfish and gastrointestinal absorption of elemental mercury from amalgams in tooth fillings. Mercury has been detected in blood,

urine, human milk, and hair in individuals in the general population. The mercury concentrations in whole blood of individuals with or without amalgam tooth fillings are usually below 5 µg/l blood, but these concentrations depend on dietary habits and the number of amalgam tooth fillings (SCENIHR, 2008). A study from Bergen in Norway, recently confirmed that the level of inorganic mercury in autopsy tissues was related to the number of dental fillings, whereas organic mercury was related to dietary intake i.e. fish intake (Björkman et al., 2007).

Levels of Hg in fish vary with species, size, age, differences in Hg exposure, food web structure, and dietary strategy. Highest concentration of mercury in fish is often found in piscivorous fish species and top predators. In Scandinavia and North America elevated concentrations of Hg is often found in Northern pike and perch, and the concentrations are often above the limit recommended for human consumption. (Ranneklev et al., 2009). In Norway a significant increase of mercury levels in trout (ca. 20 % increase) and perch (ca. 60 % increase) has been observed in 2008 compared to levels in fish caught in the period 1990 - 2001. The concentrations increase with fish size, and in average the EU maximum level of 0.5 mg Hg/kg (related to placing on the market of foodstuff) were exceeded for trout at a fish size of approximately 24 cm, or 200 g. Similar observations have been reported in Sweden. It is not known if this increase is a general trend for the EU/EEA. More detailed data on mercury levels and trends in fish is included in Appendix 8.

The following table gives an overview of the estimated intake of methylmercury from fish- and seafood product consumption in selected European countries, when consumption as well as national mercury concentration is regarded (EFSA, 2004).

Table 3.2.1: Dietary intake of methylmercury (MeHg) from fish- and seafood product consumption according to the SCOOP task 3.2.11 for countries showing high and low intakes, adapted from EFSA (2004)

	The Netherlands	Portugal	Ireland	Greece	France	Norway
National dietary exposure (µg MeHg/kg bw/week)						
Mean	<0.1	1.6	<0.1	0.5	0.3	0.4
High	-	-	0.4	2.2	-	1.8

EFSA carried out a probabilistic analysis of the likelihood of exceeding the PTWIs using the French contamination data as reported to SCOOP in combination with the distribution of fish and seafood product consumption in France (Table 3.2.2).

The probability for a population to reach an exposure above the JECFA PTWI was calculated using an empirical method, in which the individual consumption of each consumer of seafood products is multiplied by the mean level of contamination. The empirical probability is calculated as the number of subjects with an intake greater than 1.6 µg/week divided by the total number of subjects in the survey.

Table 3.2.2: Exposure assessment and probability of overstepping the tolerable intakes based on the distribution of consumption and fish contamination in France

Group	Number of subjects	Mean consumption (g/week)	Mean exposure (µg/kg bw/week)	50th percentile (µg/kg bw/week)	97.5th percentile (µg/kg bw/week)	Empirical probability of exceeding the JECFA PTWI
Children 3-6 years	293	178	0.83	0.61	3.0	11.3%
Adults 25-34 years	248	282	0.38	0.28	1.28	1.2%

According to Commission Regulation (EC) No 1881/2006 maximum levels (given as mg/kg wet weight) for certain contaminants in foodstuffs has been established (EC, 2006). A maximum level of 0.5 mg/kg mercury applies to fishery products, with the exception of certain listed fish species for which 1 mg/kg applies.

Methylmercury is highly toxic particularly to the nervous system, and the developing brain is thought to be the most sensitive target organ. The FAO/ WHO Joint Expert Committee on Food Additives (JECFA) established a provisional Tolerable Weekly Intake (PTWI) for methylmercury to 1.6 µg/kg body weight (WHO, 2003). Based on data on levels of mercury in foods in several EU countries reported by SCOOP (EC, 2004) EFSA has reported limited estimates on dietary exposure. According to SCOOP and EFSA the estimated intake of mercury in Europe varies between countries, depending on the amount and the type of fish consumed. The mean intakes were in most cases below the JECFA PTWI of 1.6 µg/kg body weight but high intakes may exceed the JECFA PTWI. Small children seem to be more likely to exceed the PTWI than adults, for details see Table 3.2.2 (EFSA, 2004).
In Norway a significant increase of mercury levels in trout (ca. 20 % increase) and perch (ca. 60 % increase) has been observed in 2008 compared to levels in fish caught in the period 1990 - 2001. The concentrations increased with fish size, and in average the EU consumption limit of 0.5 mg Hg/kg (wet weight) were exceeded for trout at a fish size of approximately 24 cm, or 200 g. Similar observations have been reported in Sweden. It is not known if this is a general trend for the EU/EEA.

The level of mercury in fish, and in particular the data indicating increasing levels in the last 10 years, is of serious concern.

3.2 Environment

3.2.1 Rationale for the risk characterization in the environment

A risk characterization should be conducted for the 5 phenyl mercury compounds by comparing the predicted concentrations in the environment (PECs) with the predicted no-effect concentrations for the compartment (PNECs). The phenylmercury compounds are degraded in the environment to give hazardous degradation products, i.e. divalent (Hg2+) and elemental (Hg0) mercury, which can be transformed to methylmercury. Consequently the risk assessment should give consideration to the risks that might arise from the degradation/transformation products as well. Due to lack of data, but also due to the fate of

the phenyl mercury compounds in the environment, it is proposed to perform the quantitative risk assessment for environment on the basis of the inorganic mercury data.
One of the main degradation / transformation products of phenylmercury compounds is methylmercury. The PBT like properties of methylmercury will override a quantitative risk assessment and a qualitative risk assessment has been performed in section B 10.2

Environmental concentrations (at regional level) have been calculated using the substance properties of phenylmercury acetate (which is the only of the compounds for which sufficient data are available), however assuming that the substance is not biodegradable (as elemental mercury was identified as the relevant component for risk assessment). This worst case release estimation was based on the total consumption volume of all compounds in terms of elemental mercury, i.e. 31.33 tonnes/year, and the distribution of releases to the environment as summarised in Section B.9.6.1.

The risk characterisation for the aquatic compartment is based on PNECs for divalent mercury because this species is expected to be the dominant species in the aquatic environment. Phenylmercury acetate is rapidly degraded in aquatic environments and methylmercury is taken into account in the qualitative risk assessment as a PBT-like compound. The risk characterisation for the terrestrial compartment is based on two-valent mercury. In soil, phenylmercury compounds are predominantly degraded to two-valent mercury, and therefore, terrestrial organisms are chronically exposed to this mercury species. Due to lack of data a quantitative risk assessment for the marine environment could not be performed.

It should be born in mind that a piece by piece risk assessment of releases of mercury and mercury compounds from single product groups does not give a comprehensive picture of the risks. For that purpose different sources of releases would have to be combined.

3.2.2 Aquatic compartment

The risk characterisation ratio is based both on freshwater and on marine assessment. As explained above the PECs calculations have been performed using the substance properties of phenylmercury acetate, however assuming that the substance is not biodegradable, as elemental mercury was identified as the relevant component for risk assessment.

Regional scenario.

Predicted environmental concentrations (PEC):
Aquatic compartment
Regional PEC, surface water (total): 0.00278 µg Hg/L
Continental PEC, surface water (total): 0.00236 µg Hg/L

Regional PEC, sea water (total) 0.0003 µg Hg/L
Continental PEC, sea water (total) 0.00004 µg Hg/L

Aquatic sediment
Regional PEC, sediment: 0.93 µg/kg wwt

Continental PEC, sediment: 0.79 µg/kg wwt

Predicted No Effect concentrations PNEC for inorganic mercury):

PNECwater.SSD = 0.047 µg Hg /L

PNEC sediment =0.47 mg Hg/kg wwt

Risk characterisation ratios:

Freshwater environment
PECsurface water, regional/PNECwater= 0.00278[µg/l]/0.047 [µg/L] = 0.06
PECsurface water, continental/PNECwater= 0.00236[µg/l]/0.047 [µg/L] = 0.05

The risk ratio for phenylmercury acetate for freshwater is 0.20 and 0.17 on the regional and continental scale, respectively.

Both for phenylmercury acetate and ionic mercury the risk ratio (PECsurface water/PNECwater) for surface water is lower than 1. This indicates that the emissions of phenylmercury compounds per se do not pose a risk on freshwater environments.

Marine environment
PECsea water, regional/PNECHg.water= 0.0003[µg/l]/0.047 [µg/L] = 0.006
PECsea water, continental/PNECHg.water= 0.00004[µg/l]/0.047 [µg/L] = 0.00085

For phenylmercury acetate, the risk ratio for sea water is 0.23 and 0.03 on the regional and continental scale, respectively.

Both for phenylmercury acetate and ionic mercury the risk ratio (PECsea water/PNECwater) for sea water is lower than 1. This indicates that the emissions of phenylmercury compounds per se do not pose a risk on marine environments.

Sediment

PECsediment.regional/PNECHg,sediment = 0.00093 [mg/kg]/0.47 [mg/kg] = 0.001
PECsediment.continental/PNECHg,sediment = 0.00079 [mg/kg]/0.47 [mg/kg] = 0.002

PECsea water sediment.regional/PNECHg,sediment = 0.000092 [mg/kg]/0.47 [mg/kg] = 0.0002
PECsea water sediment.continental/PNECHg,sediment = 0.000012 [mg/kg]/0.47 [mg/kg] = 0.00003

Therefore PECsediment/PNECsediment = <1

For ionic mercury the risk ratio (PEC(seawater) sediment/PNECsediment) for sediment is considerably lower than 1. This indicates that the emissions of phenylmercury compounds per se do not pose a risk on sediment living organisms.

In the RPA report (2002) mercury used in products like dental amalgam, batteries, lamps,

measuring and electrical equipment were evaluated but products containing phenylmercury compounds were not considered. According to the RPA report (2002) for water, the PEC/PNEC ratios for inorganic and organic mercury were significantly less than 1. For sediment, the PEC/PNEC ratios were significantly less than 1 for inorganic mercury whilst those for organic mercury were in the range of 0.2 - 0.4.

3.2.3 Terrestrial compartment

Risk characterization ratios for the terrestrial compartment can only be derived on the regional scale as exposure concentrations are solely predicted on a regional and not a local scale. In order to calculate the RCR, the PECreg, soil has to be related to dryweight. Assuming an average water content of 25% the PECreg, soil is estimated to

$$PEC_{soil,reg}\left[\frac{mg}{kg\ dw}\right] = \frac{PEC_{soil,reg}\left[\frac{mg}{kg\ wwt}\right]}{100\% - water\ content} = \frac{0.631}{0.75}\left[\frac{\mu g}{kg\ dw}\right] = 0.79\left[\frac{\mu g}{kg\ dw}\right]$$

The RCRreg, soil is calculated as

$$RCR_{soil,regional} = \frac{PEC_{soil,regional}}{PNEC_{soil}} = \frac{0.79\,\mu g\,kg^{-1}\ dw}{2.42\,\mu g\,kg^{-1}\ dw} = 0.33$$

The risk ration(RCR) of 0.33 indicates that the environmental risk of the addressed phenyl mercury compounds per se is low for the soil compartment, however, in a cumulative risk assessment environmental concentration of mercury might be high enough to pose a risk for the soil compartment.

3.2.4 Secondary poisoning

Because of lack of data a PECoral has not been calculated (neither for the phenylmercury compounds compounds themselves or the degradation products). A quantitative risk characterization for secondary poisoning could not been performed.

According to the UNEP report (2002) all forms of mercury can accumulate to some degree but methylmercury is absorbed and accumulates to a greater extent than other forms. Furthermore, the UNEP report (2002) states that the biomagnification of methylmercury has a most significant influence on the impact on animals and humans and that nearly 100 percent of mercury that bioaccumulates in predator fish is methylmercury. Most of the methylmercury that is found in fish tissues is covalently bound to protein sulfhydryl groups. This binding results in a long half-life for elimination (about two years). As a consequence, methylmercury is selectively enriched (relative to inorganic mercury) from one trophic level to the next higher trophic level.

According to the RPA report (2002) (phenylmercury containing products were not included), for secondary poisoning, the PEC/PNEC ratios were significantly less than unity (i.e. <1) for the terrestrial food chain when considering inorganic mercury whilst those for the aquatic food chain using organic mercury approached 1 (0.9). It may be assumed that organic mercury (particularly methylmercury) has the potential to cause secondary poisoning through the food chain.

This is supported by monitoring data from a study of Northern Fulmar where the levels of mercury were high compared to other Arctic seabird species. The levels were close to levels associated with malnutrition and chronic diseases in other seabird species (Gabrielsen et al., 2005).

3.2.5 Conclusions (environment)

Phenylmercury compounds are degraded in the environment to hazardous degradation products as i.e elemental mercury and divalent mercury, which can be transformed to methylmercury. Due to the PBT like properties of methymercury a quantitative risk assessment has been performed. The concentrations of inorganic mercury predicted to be in the freshwater and terrestrial environment resulting from the emissions of the phenylmercury compounds are below that predicted to cause an effect. The RPA report (2002) concluded that using the TGD/EUSES approach (with modifications), it would appear that there are unlikely to be significant risks to water, sediment and soil associated with the mercury containing products evaluated in that report. However, it was concluded that there may be effects through secondary poisoning via the aquatic food chain. It is recognised that a piece by piece risk assessment of mercury and mercury compounds from single or selected product groups does not give the full picture of the risks, for that purpose all different sources of exposure would have to be combined. It is evident that the life-cycle of the phenylmercury compounds adds to the overall emissions of mercury to the environment and thereby to the exposure of the environment.

Appendix 2. QSAR estimation of selected chemical and environmental fate properties

No data on the environmental fate and toxicity of phenylmercury propionate, 2-ethylhexanoate, octanoate and neodecanoate is available. In this case, alternative assessment methods like QSARs (Quantitative or Qualitative Structure-Activity Relationships) can be used to predict the fate of chemicals with unknown physical-chemical relationships in the environment. QSARs are models that predict the potency (quantitative) or mechanism of action (qualitative) of a substance from its chemical structure.
The QSAR approach was used to estimate the octanol-water partition coefficient (KOW) and the bioconcentration factor of the five phenylmercury compounds.
The QSAR assessment of phenylmercury compounds was mainly conducted with the estimation software EPI (Estimation Programs Interface) Suite™ (version 4.0.0) developed by US-EPA. Additionally, the (Q)SAR Application Toolbox (version 1.1.02) developed by the OECD was used to search for further information.

Estimation of the octanol-water coefficient of phenylmercury propionate, 2-ethylhexanoate, octanoate and neodecanoate

EpiSuite
The estimation of the KOW by the EpiSuite software (KOWWIN) is based on the assumption that each fragment or atom in a molecule in itself contributes to the log KOW of the compound. Log KOW is the sum of the various fragments. Generally, organometallic compounds are not covered by the applicability domain of EpiSuite KOWWIN . Therefore, it has to be investigated if the applicability domain of KOWWIN can be extracted to encompass the five phenylmercury compounds. This was done according to the methodology described in chapter “Applicability domain”.

Extraction of the applicability domain of KOWWIN
The training set used to develop the EPI suite KOWWIN model consists of 2447 chemicals. A set of other 10946 chemicals was used to validate the model. In the training and validation sets experimental values were available for four and eight mercurial chemicals, respectively.
Training chemicals were split into two subsets:
Correctly predicted chemicals – deviation between observed and predicted log Kow values was less than 0.5 log units
Incorrectly predicted chemicals - deviation between observed and predicted log Kow values was greater than 0.5 log units.

Atom centered fragments (ACFs) accounting for type of atoms, hybridization and attached H-atoms were used to characterize the molecular structure. The following rules were applied in order to determine the size of ACFs:
One bond for C{sp3} neighbors
Three bonds for sequence of the remaining atoms
If an aromatic atom was a neighbor then its aromatic ring was considered as a neighbour.

The optimal threshold for splitting fuzzy characteristics was found to be no less 0.3 corresponding on adjusted Pearson’s contingency coefficient C* = 0.89.

According to the extracted applicability domain only one chemical (phenylmercury acetate) of the five phenylmercury compounds was found to belong to the domain of KOWWIN. The remaining four chemicals were classified out of the domain due to the presence in their structures of unknown ACFs. The analysis of unknown ACFs revealed that differences of these fragments from correct ACFs consist only in alteration of H- or C{3}-atoms, and after the procedure for relaxing (augmentation) the applicability domain these chemicals could be considered in the domain of KOWWIN model.

QSAR-toolbox
The estimation performed with the OECD (Q)SAR-toolbox was done by trend analysis. The chemicals used for the estimation of the KOW of the five phenylmercury compounds were all organomercurials with experimentally determined KOW. Of 107 chemicals belonging to this group, experimental data on KOW is available for 8 of these chemicals. Trend-analysis was performed with these chemically similar chemicals, however except for phenylmercury proprionate, KOWs for the other four phenylmercury compounds were out of applicability domain. Therefore these values have to be judged cautiously.

Estimation of KOW
The log KOW values estimated by EpiSuite and the OECD-toolbox are listed in Table 2.1.

Table 2.1: Estimated octanol-water coefficients using the software EpiSuite (v. 4.0.0.) and OECD-(Q)SAR toolbox (v. 1.1.2)

Cas-nr	Substance	LogKow (Episuite)	LogKow (OECD toolbox
62-38-4	Phenylmercury acetate (PMA)	0.89 (estimated) (0.71 experimental)	1.27
103-27-5	Phenylmercury propionate	1.38	1.65
13302-00-6	(2-ethylhexanoato)phenylmercury	3.76	3.65
13864-38-5	Phenylmercuric octanoate	3.84	3.71
26545-49-3	Phenylmercury neodecanoate	4.71	4.45

Estimated and experimentally determined KOW-values are quite similar for phenylmercury acetate, the only compound where experimental data for KOW were found. The estimation with the OECD toolbox (using tested values on organometallic compounds and trend analysis) is in accordance with the estimated data from Episuite for all five phenylmercury compounds.

Estimation of the bioconcentration factor (BCF) of phenylmercury propionate, 2-ethylhexanoate, octanoate and neodecanoate
Of 71 phenylmercury compounds found in the EINECS database, experimental data is only available for phenylmercury acetate (log BCF 1,90 – 5,3) and phenylmercury hydroxide (log BCF 3,6 – 4,2). For phenylmercury acetate experimental BCFs in rainbow trout were determined to 80 – 100, while values for shrimps, algae and copepods are between 1700 and

180000). Estimation of the bioconcentration factor was performed with the EpiSuite BCFBAF model that is based on work of Meylan et al. (1997), Meylan et al. (1998) and Arnot and Gobas (2003).
For organomercurials, the BCF in fish is estimated using the Kow. Additionally a general adjustment factor is applied for compounds containing mercury and tin. For low KOWs the BCF is estimated to a fix value of 100. This means that the BCF for organomercury and organotin compounds cannot be lower than 100. For the more hydrophobic phenylmercury 2-ethylhexanoate, octanoate and neodecanoate the BCFs are estimated using the following equation:
Log BCF = 0.6598 log Kow - 0.333 + 1.4 (correction for mercury compounds)
The QSAR does not take into account biotransformation of the phenylmercury compounds, i.e. the cleavage of the esterlike bond. This results in an overestimation of the BCFs for the ethylhexanoate, octanoate and neodecanoate and should be compensated by a correction factor similar to that applied to compounds with a cyclopropyl ester group (correction factor: – 1.65). The estimated BCFs taking biotransformation into account (see table above) were calculated according to the equation
Log BCF = 0.6598 log Kow - 0.333 + 1.4 (correction for mercury compounds) – 1.65 (corr. for ester compounds).

Generally, organometallic compounds are not covered by the applicability domain of EpiSuite BCFBAF. Therefore, it has to be investigated if the applicability domain of KOWWIN can be extracted to encompass the five phenylmercury compounds. This was done according to the methodology described in chapter “Applicability domain”.

Extraction of the applicability domain of BCFBAF
The training set used to developed EPI suite BCF model includes 527 chemical (including two mercury compounds) with experimental and estimated BCF values.

Training chemicals were split into two subsets:

Correctly predicted chemicals – deviation between observed and predicted log BCF values was less than 0.75 log units
Incorrectly predicted chemicals - deviation between observed and predicted log BCF values was greater than 0.75 log units.

ACFs accounting for type of atoms, hybridization and attached H-atoms were used as characteristics of molecular structure. The following rules were applied in order to determine the size of ACFs:

One bond for C{sp3} neighbors
Three bonds for sequence of the remaining atoms
If an aromatic atom was a neighbor then its aromatic ring was considered as a neighbor.

The optimal threshold for splitting fuzzy characteristics was found to be no less 0.02 corresponding on adjusted Pearson’s contingency coefficient C* = 0.95.

According to the extracted applicability domain only one chemical (phenylmercury acetate) of the five phenylmercury compounds was found to belong to the domain of BCF model. The remaining four chemicals were classified out of the domain due to the presence in their structures of unknown ACFs. The analysis of unknown ACFs revealed that differences of

these fragments from correct ACFs consist only in alteration of H- or C{3}-atoms and according to the augmented applicability domain these chemical could be considered in the domain of BCF model.

Estimation of BCF

BCFs estimated with the BCFBAF model in EpiSuite are listed in Table 2.2. BCFs of the proposed phenylmercury compounds vary between 100 and 14890 if no biotransformation is assumed. BCFs taking biotransformation into account are between 0.9 and 225. It is known that phenylmercury acetate is rapidly biotransformed to inorganic mercury in fish (Fang, S.C., 1973). Therefore, BCFs taking biotransformation into account seem to be more realistic than those assuming persistence of phenylmercury compounds in organisms.

Table 2.2: Bioconcentration factors estimated by the BCFBAF-model in EpiSuite

Cas-nr	Substance	BCF estimated (without biotransformation)	BCF estimated (with biotransformation)
62-38-4	Phenylmercury acetate	100	0.9
103-27-5	Phenylmercury propionate	100	2.3
13302-00-6	(2-ethylhexanoato)phenylmercury	3546	70.3
13864-38-5	Phenylmercuric octanoate	3965	74.3
26545-49-3	Phenylmercury neodecanoate	14890	225

Applicability domain

The structural applicability domain of a (Q)SAR model is based on formal definition of structural similarity between chemicals in the training set and the target chemicals. In general, similarity between two objects is estimated by the number of matches or the overlap in the objects, with respect to one or more of their characteristics.

The characteristics of molecular structure can be separated into topological and chemical characteristics. The topological characteristics bring information about the atom connectivity, while the chemical characteristics provide information about the atom species, hybridization, bond type, valences, etc. Frequently used characteristics accounting for molecular topology and chemistry are as follows:

Atom pairs - substructures of the form Atomi – Atomj – Distance, where Distance is the distance in bonds along the shortest path between an atom of type Atomi and an atom of type Atomj. Atom types may encode the species of atom, the number of non-hydrogen atoms attached to it, hybridization, atom charge, etc.

Topological torsions – structures of the form Atomi – Atomj – Atomk – Atoml, where i, j, k, and l are consecutively bonded distinct atoms. Atom types encode the species of atom, the number of non-hydrogen atoms attached to it, hybridization, atom charge, etc. The bond type is explicitly encoded in the topological torsions.

Atom centred fragment - defined by molecular subfragment containing this atom and its first, second, etc. neighbours. This approach partitions the molecules into atom-centred fragments with information about species of central atom and its neighbours, hybridizations, atomic rings, valences, type of bonds, etc.
Pathways – acyclic sequences atoms (usually of 1 to 8) of the form (Atomi)n where n=1, 2, ... Atom types encode the species of atom, the number of non-hydrogen atoms attached to it, hybridization, atom charge, etc. The bond type is explicitly encoded in the sequence.
Cycles - sequences of atoms of the form Atomi-(Atomi)n- Atomi. Atom types encode the species of atom, the number of non-hydrogen atoms attached to it, hybridization, atom charge, etc. The bond type is explicitly encoded in the sequence.

The information stored in atom pairs, topological torsions and other sub-structural fragments can be encoded in fingerprints or holograms. The fingerprint is a bit-string where if a given fragment is present in the molecule a value of 1 is assigned to that position in the fingerprint, whereas if the fragment is not presented a value of 0 is assigned. Because the bits reflects only the local structural information only a poor encoding of global structural properties such as molecular size and shape is possible with fingerprints. In this respect more informative is molecular hologram. Instead of using a binary bit string containing either 0 or 1 in each bin, a molecular hologram retains a count of the number of times each fragment is set.

The reliability of a model to provide correct prediction for a certain target chemical can be estimated assuming that similar chemicals have similar activity. This assumption supposes that some measure of similarity between target chemical and training chemicals is accepted. It should be taken into account that not all chemicals used to build the model are well predicted by the model. In this respect the training chemicals can be split into two subsets:

Correct chemicals – these are chemicals that are predicted by the model with accuracy comparable with the experimental error,
Incorrect chemicals – predictions are beyond the variation of experimental error.

These two subsets of chemicals are used to extract characteristics that determine the structural space of correct and incorrect chemicals. Extracted characteristics are split into three categories: unique characteristics of correct and incorrect chemicals (presented only in one of the subsets) and fuzzy characteristics presented in both subsets of chemicals. Figure 1 illustrates this process.

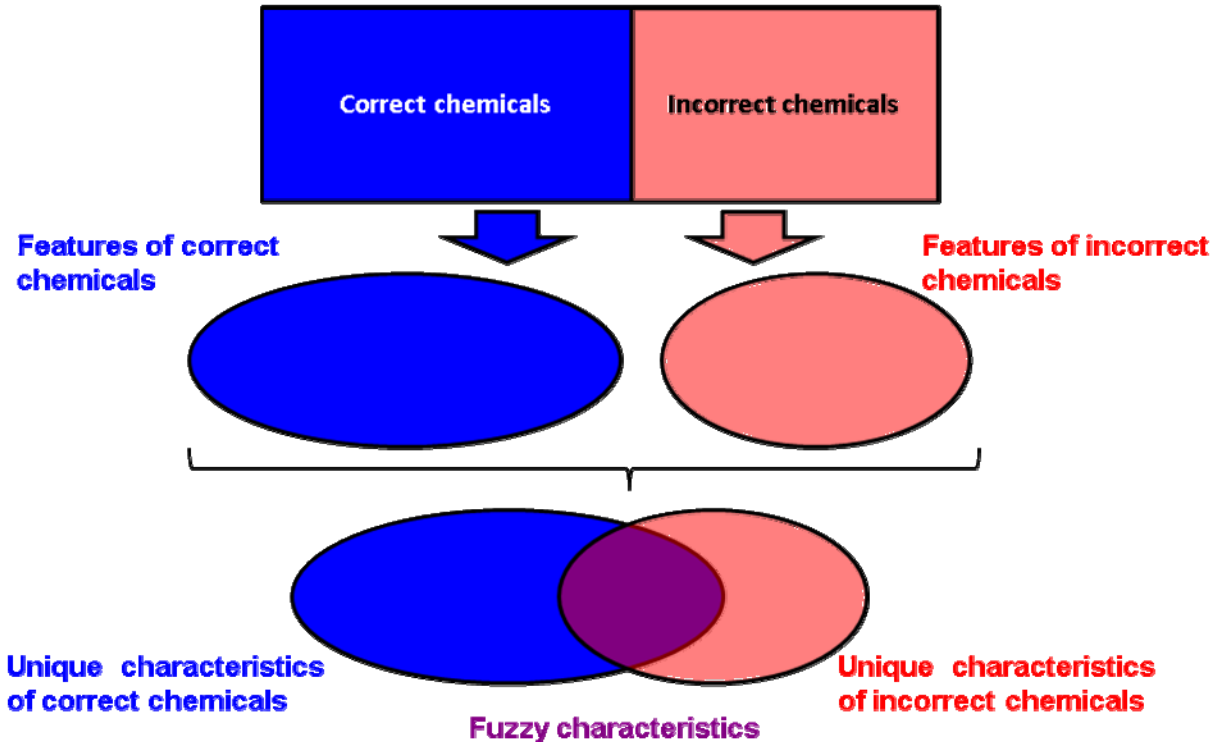


Figure 1. Characteristics of correct and incorrect chemicals.

The structural characteristics of a target chemical can belong to the following four categories:

Unique characteristics of correct chemicals,
Unique characteristics of incorrect chemicals,
Fuzzy characteristics of correct and incorrect chemicals,
Characteristics not presented in correct and incorrect chemicals, named unknown characteristics.

A chemical is classified in the model domain if the following inequalities are fulfilled:

$$w_{Corr} \geq Th_{Corr} \quad (1)$$

$$w_{Incorr} \leq Th_{Incorr} \quad (2)$$

$$w_{Unknown} \leq Th_{Unknown} \quad (3)$$

$$w_{Fuzzy} \leq Th_{Fuzzy} \quad (4)$$

$$w_i = \frac{N_i}{\sum_j N_j}$$

where (w_{Corr}, w_{Incorr}, $w_{Unknown}$ and w_{Fuzzy}) are relative frequencies of different types of characteristics of the chemical, Nj is the number characteristic of type j and Thj are corresponding user defined thresholds. According to the trivial approach a chemical is accepted to belong to the applicability domain if it is constituted by correct fragments only ($Th_{Corr} = 100$) and the remaining thresholds are accepted to be equal to zero. In this case, all

correctly predicted chemicals with at least one fuzzy characteristic will be classified as out of domain chemicals. If all fuzzy characteristics are treated as correct, then all non-correctly predicted by the model chemicals constituted by correct and fuzzy characteristics only will be classified in the model domain (false positives). It is clear that the treatment of a fuzzy fragment as correct should be based on the analysis of its effect on model predictions.

As a source of information for the effect of fuzzy fragments on the model predictions could be used their frequency of occurrence in correctly and incorrectly predicted chemicals. The selection of the optimal threshold for treatment of fuzzy characteristics in this case could be based on their distribution among correctly and incorrectly predicted chemicals:

$$w_{Corr}^{Fuzzy} = \frac{N_{Corr}}{N_{Corr} + N_{Incorr}} \quad (5)$$

$$w_{Incorr}^{Fuzzy} = 1 - w_{Corr}^{Fuzzy} = \frac{N_{Incorr}}{N_{Corr} + N_{Incorr}} \quad (6)$$

where N_{Corr} and N_{Incorr} are number of occurrence of a fuzzy fragment in correctly and incorrectly predicted by the model training chemicals, and w_{Corr}^{Fuzzy} and w_{Incorr}^{Fuzzy} are relative frequencies of occurrence in both type of chemicals, respectively. A fuzzy fragment is assumed to belong to e set of correct characteristics if its relative frequency w_{Corr}^{Fuzzy} is greater than some predefined threshold:

$$w_{Corr}^{Fuzzy} \geq Th_{Corr}^{Fuzzy} . \quad (7)$$

The optimal value of the threshold Th_{Corr}^{Fuzzy} should provide the best classification of training chemicals. As an objective function is proposed to be used the adjusted Pearson's contingency coefficient C*:

$$\max_{Th_{Corr}^{Fuzzy} \in [0,1]} : C^* \quad (8)$$

Although optimization defined by Eq. 8 is a non-linear problem the solution could be easily found with a simple incremental method because C* is one variable objective function and the range of variation of its independent variable (Th_{Corr}^{Fuzzy}) is within the interval [0, 1].

EpiSuite reports

Phenylmercury acetate

CAS Number: 62-38-4
SMILES : CC(=O)O[Hg]c1ccccc1
CHEM : Phenylmercuric acetate
MOL FOR: C8 H8 O2 Hg1
MOL WT : 336.74
---------- EPI SUMMARY (v4.00) ----------

Physical Property Inputs:
Log Kow (octanol-water): 0.71
Boiling Point (deg C) : ------
Melting Point (deg C) : 150.00
Vapor Pressure (mm Hg) : 6E-006
Water Solubility (mg/L): 4370
Henry LC (atm-m3/mole) : 5.66E-010

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.67 estimate) = 0.89
Log Kow (Exper. database match) = 0.71
Exper. Ref: HANSCH,C ET AL. (1995)

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 290.77 (Adapted Stein & Brown method)
Melting Pt (deg C): 65.81 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 0.00017 (Modified Grain method)
VP (Pa, 25 deg C) : 0.0227 (Modified Grain method)
MP (exp database): 153 deg C
VP (exp database): 6.00E-06 mm Hg (8.00E-004 Pa) at 20 deg C
Subcooled liquid VP: 0.000103 mm Hg (20 deg C, user-entered VP)
: 0.0138 Pa (20 deg C, user-entered VP)

Water Solubility Estimate from Log Kow (WSKOW v1.41):
Water Solubility at 25 deg C (mg/L): 2145
log Kow used: 0.71 (user entered)
melt pt used: 150.00 deg C
Water Sol (Exper. database match) = 4370 mg/L (15 deg C)
Exper. Ref: TOMLIN,C (1994)

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 1164.7 mg/L

ECOSAR Class Program (ECOSAR v1.00):
Class(es) found:
Neutral Organics

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:

Bond Method : 5.87E-010 atm-m3/mole (5.95E-005 Pa-m3/mole)
Group Method: Incomplete
Exper Database: 5.66E-10 atm-m3/mole (5.73E-005 Pa-m3/mole)
For Henry LC Comparison Purposes:
User-Entered Henry LC: 5.660E-010 atm-m3/mole (5.735E-005 Pa-m3/mole)
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 6.083E-010 atm-m3/mole (6.164E-005 Pa-m3/mole)
VP: 6E-006 mm Hg (source: User-Entered)
WS: 4.37E+003 mg/L (source: User-Entered)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: 0.71 (user entered)
Log Kaw used: -7.636 (user entered)
Log Koa (KOAWIN v1.10 estimate): 8.346
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.7153
Biowin2 (Non-Linear Model) : 0.5065
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.4770 (weeks-months)
Biowin4 (Primary Survey Model) : 3.3668 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : -0.2482
Biowin6 (MITI Non-Linear Model): 0.0014
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.4975
Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):
Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 0.0137 Pa (0.000103 mm Hg)
Log Koa (Koawin est): 8.346
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 0.000218
Octanol/air (Koa) model: 5.45E-005
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 0.00783
Mackay model : 0.0172
Octanol/air (Koa) model: 0.00434

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 1.9920 E-12 cm3/molecule-sec
Half-Life = 5.369 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 64.434 Hrs
Ozone Reaction:
No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):
0.0125 (Junge-Pankow, Mackay avg)
0.00434 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc : 56.44 L/kg (MCI method)
Log Koc: 1.752 (MCI method)
Koc : 12.26 L/kg (Kow method)
Log Koc: 1.089 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.00):
Log BCF from regression-based method = 2.000 (BCF = 100 L/kg wet-wt)
Log Biotransformation Half-life (HL) = -1.6363 days (HL = 0.0231 days)
Log BCF Arnot-Gobas method (upper trophic) = 0.061 (BCF = 1.15)
Log BAF Arnot-Gobas method (upper trophic) = 0.061 (BAF = 1.15)
log Kow used: 0.71 (user entered)

Volatilization from Water:
Henry LC: 5.66E-010 atm-m3/mole (entered by user)
Half-Life from Model River: 1.898E+006 hours (7.909E+004 days)
Half-Life from Model Lake : 2.071E+007 hours (8.628E+005 days)

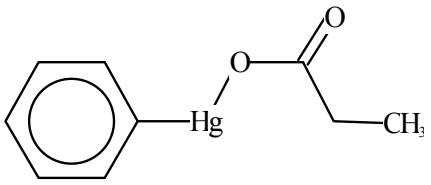
Removal In Wastewater Treatment:
Total removal: 1.87 percent
Total biodegradation: 0.09 percent
Total sludge adsorption: 1.77 percent
Total to Air: 0.00 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.00952	129	0.71
Water	3.38	900	0.034
Soil	95	1.8e+003	0
Sediment	1.64	8.1e+003	0

Persistence Time: 2.33e+003 hr

Phenylmercury propionate



SMILES : c1([Hg]OC(=O)CC)ccccc1
CHEM :
MOL FOR: C9 H10 O2 Hg1
MOL WT : 350.77
---------- EPI SUMMARY (v4.00) ----------
Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------

KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): 1.38

SMILES : c1([Hg]OC(=O)CC)ccccc1
CHEM :
MOL FOR: C9 H10 O2 Hg1
MOL WT : 350.77

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	0.5473	0.5473
Frag	1	-CH2- [aliphatic carbon]	0.4911	0.4911
Frag	6	Aromatic Carbon	0.2940	1.7640
Frag	1	-C(=O)O [ester, aliphatic attach]	-0.9505	-0.9505
Frag	1	-Hg- [mercury]	-0.7000	-0.7000
Const		Equation Constant		0.2290

Log Kow = 1.3809

MPBPVP (v1.43) Program Results:
==========
Experimental Database Structure Match: no data

SMILES : c1([Hg]OC(=O)CC)ccccc1
CHEM :
MOL FOR: C9 H10 O2 Hg1
MOL WT : 350.77
---------- SUMMARY MPBVP v1.43 ----------

Boiling Point: 305.56 deg C (Adapted Stein and Brown Method)

Melting Point: 86.78 deg C (Adapted Joback Method)
Melting Point: 64.75 deg C (Gold and Ogle Method)
Mean Melt Pt : 75.77 deg C (Joback; Gold,Ogle Methods)
Selected MP: 75.77 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 305.56 deg C (estimated))
(Using MP: 75.77 deg C (estimated))
VP: 0.000357 mm Hg (Antoine Method)
: 0.0476 Pa (Antoine Method)
VP: 0.000479 mm Hg (Modified Grain Method)
: 0.0639 Pa (Modified Grain Method)
VP: 0.000867 mm Hg (Mackay Method)
: 0.116 Pa (Mackay Method)
Selected VP: 0.000479 mm Hg (Modified Grain Method)
: 0.0639 Pa (Modified Grain Method)
Subcooled liquid VP: 0.00145 mm Hg (25 deg C, Mod-Grain method)
: 0.194 Pa (25 deg C, Mod-Grain method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	1	-CH3	21.98	21.98
Group	1	-CH2-	24.22	24.22
Group	1	-COO- (ester)	78.85	78.85
Group	5	CH (aromatic)	28.53	142.65
Group	1	-C (aromatic)	30.76	30.76
Group	1	Mercury	130.00	130.00
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		626.64
RESULT- corr		BOILING POINT in deg Kelvin		578.72
		BOILING POINT in deg C		305.56

```
-------+-----+--------------------+----------+---------
TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
Group |  1  |  -CH3              |   -5.10  |   -5.10
Group |  1  |  -CH2-             |   11.27  |   11.27
Group |  1  |  -COO- (ester)     |   53.60  |   53.60
Group |  5  |  CH (aromatic)     |    8.13  |   40.65
Group |  1  |  -C (aromatic)     |   37.02  |   37.02
Group |  1  |  Mercury           |  100.00  |  100.00
*  |    |  Equation Constant |          |  122.50
============+====================+==========+=========
RESULT    |  MELTING POINT in deg Kelvin  |  359.94
|  MELTING POINT in deg C       |   86.78
-----------------------------------------------------
```

Water Sol from Kow (WSKOW v1.41) Results:
==========

Water Sol: 405.6 mg/L

SMILES : c1([Hg]OC(=O)CC)ccccc1
CHEM :
MOL FOR: C9 H10 O2 Hg1
MOL WT : 350.77
---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : 1.38
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 1.38

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s): Value
---------- -----
No Applicable Correction Factors

Log Water Solubility (in moles/L) : -2.937
Water Solubility at 25 deg C (mg/L): 405.6

WATERNT Program (v1.01) Results:
==========

Water Sol (v1.01 est): 352.31 mg/L

SMILES : c1([Hg]OC(=O)CC)ccccc1

CHEM :
MOL FOR: C9 H10 O2 Hg1
MOL WT : 350.77

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	-0.3213	-0.3213
Frag	1	-CH2- [aliphatic carbon]	-0.5370	-0.5370
Frag	5	Aromatic Carbon (C-H type)	-0.3359	-1.6793
Frag	1	-C(=O)O [ester, aliphatic attach]	0.5757	0.5757
Frag	1	Aromatic Carbon (C-substituent type)	-0.5400	-0.5400
Frag	1	-Hg- [mercury]	-0.7455	-0.7455
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -2.9981
Water Solubility (mg/L) at 25 dec C = 352.31

HENRYWIN (v3.20) Program Results:
==========

Bond Est : 7.80E-010 atm-m3/mole (7.90E-005 Pa-m3/mole)
Group Est: Incomplete

SMILES : c1([Hg]OC(=O)CC)ccccc1
CHEM :
MOL FOR: C9 H10 O2 Hg1
MOL WT : 350.77

---------- HENRYWIN v3.20 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	5 Hydrogen to Carbon (aliphatic) Bonds		-0.5984
HYDROGEN	5 Hydrogen to Carbon (aromatic) Bonds		-0.7715
FRAGMENT	1 C-C		0.1163
FRAGMENT	1 C-CO		1.7057
FRAGMENT	6 Car-Car		1.5828
FRAGMENT	1 CO-O		0.0714
FRAGMENT	1 Car-Hg	ESTIMATE	0.8900
FRAGMENT	1 O-Hg	ESTIMATE	4.5000
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	7.496

HENRYs LAW CONSTANT at 25 deg C = 7.80E-010 atm-m3/mole
= 3.19E-008 unitless
= 7.90E-005 Pa-m3/mole

```
|      GROUP CONTRIBUTION DESCRIPTION        |  COMMENT  |  VALUE
--------+-------------------------------------------+-----------+--------
|         1  CH3 (X)                    |           | -0.62
|         1  CH2 (C)(CO)                |           | -0.15
|         5  Car-H (Car)(Car)           |           |  0.55
|         1  CO (C)(O)                  |           |  4.09
|           MISSING Value for:  Car (Car)(Hg)(Car)
|           MISSING Value for:  UNTYPED(O)(Car)
|           MISSING Value for:  O (CO)(Hg)
--------+-------------------------------------------+-----------+--------
RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  |
INCOMPLETE |  3.87
--------+-------------------------------------------+-----------+--------
```

For Henry LC Comparison Purposes:
Exper Database: none available
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 5.451E-007 atm-m3/mole (5.523E-002 Pa-m3/mole)
VP: 0.000479 mm Hg (source: MPBPVP)
WS: 406 mg/L (source: WSKOWWIN)

Log Octanol-Air (KOAWIN v1.10) Results:
==========

Log Koa: 8.876

SMILES : c1([Hg]OC(=O)CC)ccccc1
CHEM   :
MOL FOR: C9 H10 O2 Hg1
MOL WT : 350.77
---------- KOAWIN v1.10 Results ----------

Log Koa (octanol/air) estimate: 8.876
Koa (octanol/air) estimate: 7.522e+008
Using:
Log Kow: 1.38 (KowWin est)
HenryLC: 7.8e-010 atm-m3/mole (HenryWin est)
Log Kaw: -7.496 (air/water part.coef.)

LogKow : ---- (exp database)
LogKow : 1.38 (KowWin estimate)
Henry LC: --- atm-m3/mole(exp database)
Henry LC: 7.8e-010 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate: 8.876 (from KowWin/HenryWin)

AEROWIN Program (v1.00) Results:
==========
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 0.193 Pa (0.00145 mm Hg)
Log Koa (Koawin est): 8.876
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 1.55E-005
Octanol/air (Koa) model: 0.000185
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 0.00056
Mackay model : 0.00124
Octanol/air (Koa) model: 0.0145

AOP Program (v1.92) Results:
==========
SMILES : c1([Hg]OC(=O)CC)ccccc1
CHEM :
MOL FOR: C9 H10 O2 Hg1
MOL WT : 350.77
---------- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) --------
Hydrogen Abstraction = 0.4568 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 1.9498 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 2.4067 E-12 cm3/molecule-sec
HALF-LIFE = 4.444 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 53.332 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches
Fraction sorbed to airborne particulates (phi):
0.0009 (Junge-Pankow, Mackay avg)
0.0145 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

BCFBAF Program (v3.00) Results:
==========
SMILES : c1([Hg]OC(=O)CC)ccccc1
CHEM :

MOL FOR: C9 H10 O2 Hg1
MOL WT : 350.77
---------- BCFBAF v3.00 ----------
Summary Results:
Log BCF (regression-based estimate): 2.00 (BCF = 100 L/kg wet-wt)
Biotransformation Half-Life (days) : 0.0361 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 0.36 (BAF = 2.28 L/kg wet-wt)

Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 1.38

Equation Used to Make BCF estimate:
Log BCF = 0.6598 log Kow - 0.333 + Correction

Correction(s): Value
Tin or Mercury compound 1.400
Minimum Mercury and Tin Log BCF of 2.0 applied

Estimated Log BCF = 2.000 (BCF = 100 L/kg wet-wt)

==========
Whole Body Primary Biotransformation Rate Estimate for Fish:
==========

TYPE	NUM	LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Unsubstituted phenyl group (C6H5-)	-0.6032	-0.6032
Frag	5	Aromatic-H	0.2664	1.3319
Frag	1	Methyl [-CH3]	0.2451	0.2451
Frag	1	-CH2- [linear]	0.0242	0.0242
Frag	1	Benzene	-0.4277	-0.4277
L Kow	*	Log Kow = 1.38 (KowWin estimate)	0.3073	0.4244
MolWt	*	Molecular Weight Parameter		-0.8995
Const	*	Equation Constant		-1.5058
RESULT		LOG Bio Half-Life (days)		-1.4419
RESULT		Bio Half-Life (days)		0.03615
NOTE		Bio Half-Life Normalized to 10 g fish at 15 deg C		

Biotransformation Rate Constant:
kM (Rate Constant): 19.17 /day (10 gram fish)
kM (Rate Constant): 10.78 /day (100 gram fish)
kM (Rate Constant): 6.063 /day (1 kg fish)
kM (Rate Constant): 3.41 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):

Estimated Log BCF (upper trophic) = 0.357 (BCF = 2.277 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 0.357 (BAF = 2.277 L/kg wet-wt)
Estimated Log BCF (mid trophic) = 0.324 (BCF = 2.108 L/kg wet-wt)
Estimated Log BAF (mid trophic) = 0.324 (BAF = 2.108 L/kg wet-wt)
Estimated Log BCF (lower trophic) = 0.308 (BCF = 2.032 L/kg wet-wt)
Estimated Log BAF (lower trophic) = 0.308 (BAF = 2.032 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = 0.540 (BCF = 3.464 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 0.545 (BAF = 3.505 L/kg wet-wt)

Volatilization From Water
==========

Chemical Name:

Molecular Weight : 350.77 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 7.8E-010 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05

HALF-LIFE (hours) :	1.406E+006	1.534E+007
HALF-LIFE (days) :	5.858E+004	6.39E+005
HALF-LIFE (years) :	160.4	1750

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========
(using 10000 hr Bio P,A,S)
PROPERTIES OF:

Molecular weight (g/mol)	350.77
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	7.8E-010
Air-water partition coefficient	3.18997E-008
Octanol-water partition coefficient (Kow)	23.9883

Log Kow 1.38
Biomass to water partition coefficient 5.59767
Temperature [deg C] 25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
-Primary tank 0.01 110.71 10000.00
-Aeration tank 0.01 110.71 10000.00
-Settling tank 0.01 110.71 10000.00

STP Overall Chemical Mass Balance:
---
g/h mol/h percent

Influent 1.00E+001 2.9E-002 100.00

Primary sludge 3.07E-002 8.7E-005 0.31
Waste sludge 1.54E-001 4.4E-004 1.54
Primary volatilization 4.25E-007 1.2E-009 0.00
Settling volatilization 1.16E-006 3.3E-009 0.00
Aeration off gas 2.85E-006 8.1E-009 0.00

Primary biodegradation 1.77E-003 5.1E-006 0.02
Settling biodegradation 5.31E-004 1.5E-006 0.01
Aeration biodegradation 6.99E-003 2.0E-005 0.07

Final water effluent 9.81E+000 2.8E-002 98.06

Total removal 1.94E-001 5.5E-004 1.94
Total biodegradation 9.30E-003 2.7E-005 0.09

Level III Fugacity Model (Full-Output):
==========
Chem Name :
Molecular Wt: 350.77
Henry's LC : 7.8e-010 atm-m3/mole (Henrywin program)
Vapor Press : 0.000479 mm Hg (Mpbpwin program)
Liquid VP : 0.00152 mm Hg (super-cooled)
Melting Pt : 75.8 deg C (Mpbpwin program)
Log Kow : 1.38 (Kowwin program)
Soil Koc : 108 (KOCWIN MCI method)

Mass Amount Half-Life Emissions
(percent) (hr) (kg/hr)
Air 0.00656 107 1000
Water 16.9 900 1000
Soil 83 1.8e+003 1000
Sediment 0.12 8.1e+003 0

Fugacity Reaction Advection Reaction Advection
(atm) (kg/hr) (kg/hr) (percent) (percent)

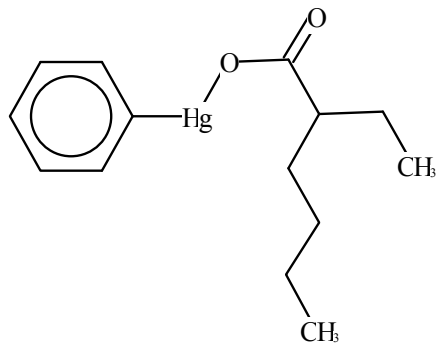
Air	2.21e-013	2.06	3.18	0.0688	0.106
Water	9.09e-015	630	818	21	27.3
Soil	1.72e-013	1.55e+003	0	51.6	0
Sediment	9.01e-015	0.497	0.116	0.0166	0.00387

Persistence Time: 1.61e+003 hr
Reaction Time: 2.22e+003 hr
Advection Time: 5.9e+003 hr
Percent Reacted: 72.6
Percent Advected: 27.4

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 106.7
Water: 900
Soil: 1800
Sediment: 8100
Biowin estimate: 2.446 (weeks-months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Phenylmercury 2-ethylhexanoate



SMILES : [Hg](OC(=O)C(CC)CCCC)c(ccc1)cc1
CHEM : Mercury, (2-ethylhexanoato-O)phenyl-
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90
---------- EPI SUMMARY (v4.00) ----------
Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------

KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): 3.76

SMILES : [Hg](OC(=O)C(CC)CCCC)c(ccc1)cc1
CHEM : Mercury, (2-ethylhexanoato-O)phenyl-
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3 [aliphatic carbon]	0.5473	1.0946
Frag	4	-CH2- [aliphatic carbon]	0.4911	1.9644
Frag	1	-CH [aliphatic carbon]	0.3614	0.3614
Frag	6	Aromatic Carbon	0.2940	1.7640
Frag	1	-C(=O)O [ester, aliphatic attach]	-0.9505	-0.9505
Frag	1	-Hg- [mercury]	-0.7000	-0.7000
Const		Equation Constant		0.2290

Log Kow = 3.7629

MPBPVP (v1.43) Program Results:
==========
Experimental Database Structure Match: no data

SMILES : [Hg](OC(=O)C(CC)CCCC)c(ccc1)cc1
CHEM : Mercury, (2-ethylhexanoato-O)phenyl-
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90
---------- SUMMARY MPBVP v1.43 ----------

Boiling Point: 360.79 deg C (Adapted Stein and Brown Method)

Melting Point: 128.13 deg C (Adapted Joback Method)
Melting Point: 97.00 deg C (Gold and Ogle Method)
Mean Melt Pt : 112.57 deg C (Joback; Gold,Ogle Methods)
Selected MP: 112.57 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 360.79 deg C (estimated))
(Using MP: 112.57 deg C (estimated))
VP: 4.05E-006 mm Hg (Antoine Method)
: 0.00054 Pa (Antoine Method)
VP: 1E-005 mm Hg (Modified Grain Method)
: 0.00134 Pa (Modified Grain Method)
VP: 1.99E-005 mm Hg (Mackay Method)
: 0.00265 Pa (Mackay Method)
Selected VP: 1E-005 mm Hg (Modified Grain Method)
: 0.00134 Pa (Modified Grain Method)
Subcooled liquid VP: 7.31E-005 mm Hg (25 deg C, Mod-Grain method)
: 0.00975 Pa (25 deg C, Mod-Grain method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	2	-CH3	21.98	43.96
Group	4	-CH2-	24.22	96.88
Group	1	>CH-	11.86	11.86
Group	1	-COO- (ester)	78.85	78.85
Group	5	CH (aromatic)	28.53	142.65
Group	1	-C (aromatic)	30.76	30.76
Group	1	Mercury	130.00	130.00
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		733.14
RESULT- corr		BOILING POINT in deg Kelvin		633.95
		BOILING POINT in deg C		360.79

```
-------+-----+-------------------+----------+---------
TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+-------------------+----------+---------
Group |  2  |  -CH3              |   -5.10  |  -10.20
Group |  4  |  -CH2-             |   11.27  |   45.08
Group |  1  |  >CH-              |   12.64  |   12.64
Group |  1  |  -COO- (ester)     |   53.60  |   53.60
Group |  5  |  CH (aromatic)     |    8.13  |   40.65
Group |  1  |  -C (aromatic)     |   37.02  |   37.02
Group |  1  |  Mercury           |  100.00  |  100.00
*   |     |  Equation Constant |          |  122.50
=============+====================+==========+=========
RESULT    |  MELTING POINT in deg Kelvin  |  401.29
          |  MELTING POINT in deg C       |  128.13
-----------------------------------------------------
```

Water Sol from Kow (WSKOW v1.41) Results:
==========

Water Sol: 1.388 mg/L

SMILES : [Hg](OC(=O)C(CC)CCCC)c(ccc1)cc1
CHEM : Mercury, (2-ethylhexanoato-O)phenyl-
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90
---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : 3.76
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 3.76

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s): Value
---------- -----
No Applicable Correction Factors

Log Water Solubility (in moles/L) : -5.482
Water Solubility at 25 deg C (mg/L): 1.388

WATERNT Program (v1.01) Results:
==========

Water Sol (v1.01 est): 1.463 mg/L

SMILES : [Hg](OC(=O)C(CC)CCCC)c(ccc1)cc1
CHEM : Mercury, (2-ethylhexanoato-O)phenyl-
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3 [aliphatic carbon]	-0.3213	-0.6425
Frag	4	-CH2- [aliphatic carbon]	-0.5370	-2.1481
Frag	1	-CH [aliphatic carbon]	-0.5285	-0.5285
Frag	5	Aromatic Carbon (C-H type)	-0.3359	-1.6793
Frag	1	-C(=O)O [ester, aliphatic attach]	0.5757	0.5757
Frag	1	Aromatic Carbon (C-substituent type)	-0.5400	-0.5400
Frag	1	-Hg- [mercury]	-0.7455	-0.7455
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -5.4589
Water Solubility (mg/L) at 25 dec C = 1.463

HENRYWIN (v3.20) Program Results:
==========

Bond Est : 3.22E-009 atm-m3/mole (3.26E-004 Pa-m3/mole)
Group Est: Incomplete

SMILES : [Hg](OC(=O)C(CC)CCCC)c(ccc1)cc1
CHEM : Mercury, (2-ethylhexanoato-O)phenyl-
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90

---------- HENRYWIN v3.20 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	15 Hydrogen to Carbon (aliphatic) Bonds		-1.7952
HYDROGEN	5 Hydrogen to Carbon (aromatic) Bonds		-0.7715
FRAGMENT	6 C-C		0.6978
FRAGMENT	1 C-CO		1.7057
FRAGMENT	6 Car-Car		1.5828
FRAGMENT	1 CO-O		0.0714
FRAGMENT	1 Car-Hg	ESTIMATE	0.8900
FRAGMENT	1 O-Hg	ESTIMATE	4.5000
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	6.881

HENRYs LAW CONSTANT at 25 deg C = 3.22E-009 atm-m3/mole

= 1.31E-007 unitless
= 3.26E-004 Pa-m3/mole

```
--------+-------------------------------------------+-----------+--------
|       GROUP CONTRIBUTION DESCRIPTION        |  COMMENT  |  VALUE
--------+-------------------------------------------+-----------+--------
|         1  CH (C)(C)(CO)                 |  ESTIMATE  |  0.13
|         2  CH3 (X)                     |          | -1.24
|         4  CH2 (C)(C)                    |          | -0.60
|         5  Car-H (Car)(Car)              |          |  0.55
|         1  CO (C)(O)                     |          |  4.09
|           MISSING Value for:  UNTYPED(O)(Car)
|           MISSING Value for:  O (CO)(Hg)
|           MISSING Value for:  Car (Car)(Car)(Hg)
--------+-------------------------------------------+-----------+--------
RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  |
INCOMPLETE |  2.93
--------+-------------------------------------------+-----------+--------
```

For Henry LC Comparison Purposes:
Exper Database: none available
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 3.990E-006 atm-m3/mole (4.043E-001 Pa-m3/mole)
VP: 1E-005 mm Hg (source: MPBPVP)
WS: 1.39 mg/L (source: WSKOWWIN)

Log Octanol-Air (KOAWIN v1.10) Results:
==========

Log Koa: 10.641

SMILES : [Hg](OC(=O)C(CC)CCCC)c(ccc1)cc1
CHEM   : Mercury, (2-ethylhexanoato-O)phenyl-
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90
---------- KOAWIN v1.10 Results ----------

Log Koa (octanol/air) estimate: 10.641
Koa (octanol/air) estimate: 4.371e+010
Using:
Log Kow: 3.76 (KowWin est)
HenryLC: 3.22e-009 atm-m3/mole (HenryWin est)
Log Kaw: -6.881 (air/water part.coef.)

LogKow : ---- (exp database)
LogKow : 3.76 (KowWin estimate)

Henry LC: --- atm-m3/mole(exp database)
Henry LC: 3.22e-009 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate: 10.641 (from KowWin/HenryWin)

AEROWIN Program (v1.00) Results:
==========
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 0.00975 Pa (7.31E-005 mm Hg)
Log Koa (Koawin est): 10.641
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 0.000308
Octanol/air (Koa) model: 0.0107
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 0.011
Mackay model : 0.024
Octanol/air (Koa) model: 0.462

AOP Program (v1.92) Results:
==========
SMILES : [Hg](OC(=O)C(CC)CCCC)c(ccc1)cc1
CHEM : Mercury, (2-ethylhexanoato-O)phenyl-
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90
---------- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) --------
Hydrogen Abstraction = 6.3682 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 1.9498 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 8.3180 E-12 cm3/molecule-sec
HALF-LIFE = 1.286 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 15.431 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches
Fraction sorbed to airborne particulates (phi):
0.0175 (Junge-Pankow, Mackay avg)
0.462 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

KOCWIN Program (v2.00) Results:
==========
SMILES : [Hg](OC(=O)C(CC)CCCC)c(ccc1)cc1
CHEM : Mercury, (2-ethylhexanoato-O)phenyl-
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90
---------- KOCWIN v2.00 Results ----------

Koc Estimate from MCI:

First Order Molecular Connectivity Index ..... : 8.274
Non-Corrected Log Koc (0.5213 MCI + 0.60) ..... : 4.9132
Fragment Correction(s):
1 Misc (C=O) Group (aliphatic attach).... : -1.6047
Corrected Log Koc ..... : 3.3086

Estimated Koc: 2035 L/kg <==========

Koc Estimate from Log Kow:

Log Kow (Kowwin estimate) ..... : 3.76
Non-Corrected Log Koc (0.55313 logKow + 0.9251) .... : 3.0049
Fragment Correction(s):
1 Misc (C=O) Group (aliphatic attach).... : -0.2293
Corrected Log Koc ..... : 2.7756

Estimated Koc: 596.5 L/kg <==========

BCFBAF Program (v3.00) Results:
==========
SMILES : [Hg](OC(=O)C(CC)CCCC)c(ccc1)cc1
CHEM : Mercury, (2-ethylhexanoato-O)phenyl-
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90
---------- BCFBAF v3.00 ----------
Summary Results:
Log BCF (regression-based estimate): 3.55 (BCF = 3.55e+003 L/kg wet-wt)
Biotransformation Half-Life (days) : 0.187 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 1.85 (BAF = 70.3 L/kg wet-wt)

Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 3.76

Equation Used to Make BCF estimate:
Log BCF = 0.6598 log Kow - 0.333 + Correction

Correction(s): Value
Tin or Mercury compound 1.400

Estimated Log BCF = 3.550 (BCF = 3546 L/kg wet-wt)

==========
Whole Body Primary Biotransformation Rate Estimate for Fish:
==========

TYPE	NUM	LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Linear C4 terminal chain [CCC-CH3]	0.0341	0.0341
Frag	1	Unsubstituted phenyl group (C6H5-)	-0.6032	-0.6032
Frag	5	Aromatic-H	0.2664	1.3319
Frag	2	Methyl [-CH3]	0.2451	0.4902
Frag	4	-CH2- [linear]	0.0242	0.0967
Frag	1	-CH- [linear]	-0.1912	-0.1912
Frag	1	Benzene	-0.4277	-0.4277
L Kow	*	Log Kow = 3.76 (KowWin estimate)	0.3073	1.1565
MolWt	*	Molecular Weight Parameter		-1.0793
Const	*	Equation Constant		-1.5058
RESULT		LOG Bio Half-Life (days)		-0.7291
RESULT		Bio Half-Life (days)		0.1866
NOTE		Bio Half-Life Normalized to 10 g fish at 15 deg C		

Biotransformation Rate Constant:
kM (Rate Constant): 3.715 /day (10 gram fish)
kM (Rate Constant): 2.089 /day (100 gram fish)
kM (Rate Constant): 1.175 /day (1 kg fish)
kM (Rate Constant): 0.6606 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) = 1.847 (BCF = 70.34 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 1.847 (BAF = 70.34 L/kg wet-wt)
Estimated Log BCF (mid trophic) = 1.932 (BCF = 85.51 L/kg wet-wt)
Estimated Log BAF (mid trophic) = 1.932 (BAF = 85.57 L/kg wet-wt)
Estimated Log BCF (lower trophic) = 1.951 (BCF = 89.24 L/kg wet-wt)
Estimated Log BAF (lower trophic) = 1.954 (BAF = 89.9 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = 2.784 (BCF = 608.2 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 3.026 (BAF = 1063 L/kg wet-wt)

Volatilization From Water
==========

Chemical Name: Mercury, (2-ethylhexanoato-O)phenyl-

Molecular Weight : 420.90 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 3.22E-009 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05

HALF-LIFE (hours) :	3.73E+005	4.07E+006
HALF-LIFE (days) :	1.554E+004	1.696E+005
HALF-LIFE (years) :	42.55	464.3

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========

(using 10000 hr Bio P,A,S)
PROPERTIES OF: Mercury, (2-ethylhexanoato-O)phenyl-

Molecular weight (g/mol)	420.9
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	3.22E-009
Air-water partition coefficient	1.31688E-007
Octanol-water partition coefficient (Kow)	5754.4
Log Kow	3.76
Biomass to water partition coefficient	1151.68
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.00	6972.78	10000.00
-Aeration tank	0.00	6972.78	10000.00
-Settling tank	0.00	6972.78	10000.00

STP Overall Chemical Mass Balance:
---

	g/h	mol/h	percent
Influent	1.00E+001	2.4E-002	100.00
Primary sludge	1.14E+000	2.7E-003	11.42

Waste sludge	8.75E-001	2.1E-003	8.75
Primary volatilization	1.43E-006	3.4E-009	0.00
Settling volatilization	3.81E-006	9.1E-009	0.00
Aeration off gas	9.39E-006	2.2E-008	0.00
Primary biodegradation	4.71E-003	1.1E-005	0.05
Settling biodegradation	1.38E-003	3.3E-006	0.01
Aeration biodegradation	1.82E-002	4.3E-005	0.18
Final water effluent	7.96E+000	1.9E-002	79.58
Total removal	2.04E+000	4.9E-003	20.42
Total biodegradation	2.43E-002	5.8E-005	0.24

Level III Fugacity Model (Full-Output):
==========

Chem Name : Mercury, (2-ethylhexanoato-O)phenyl-
Molecular Wt: 420.9
Henry's LC : 3.22e-009 atm-m3/mole (Henrywin program)
Vapor Press : 1e-005 mm Hg (Mpbpwin program)
Liquid VP : 7.35e-005 mm Hg (super-cooled)
Melting Pt : 113 deg C (Mpbpwin program)
Log Kow : 3.76 (Kowwin program)
Soil Koc : 2.04e+003 (KOCWIN MCI method)

Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air 0.0232	30.9	1000
Water 11.5	900	1000
Soil 87.2	1.8e+003	1000
Sediment 1.32	8.1e+003	0

Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air 7.29e-013	28.5	12.7	0.951	0.424
Water 2.4e-014	484	629	16.1	21
Soil 4.13e-014	1.84e+003	0	61.3	0
Sediment 2.78e-014	6.2	1.45	0.207	0.0483

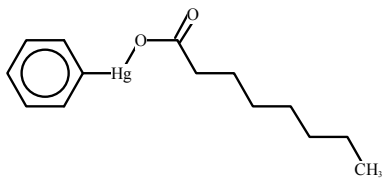
Persistence Time: 1.83e+003 hr
Reaction Time: 2.32e+003 hr
Advection Time: 8.52e+003 hr
Percent Reacted: 78.6
Percent Advected: 21.4

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 30.86
Water: 900
Soil: 1800

Sediment: 8100
Biowin estimate: 2.589 (weeks-months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Phenylmercury octanoate



SMILES : c1([Hg]OC(=O)CCCCCCC)ccccc1
CHEM :
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90
---------- EPI SUMMARY (v4.00) ----------
Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------

KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): 3.84

SMILES : c1([Hg]OC(=O)CCCCCCC)ccccc1
CHEM :
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE

```
Frag  |  1  |  -CH3    [aliphatic carbon]              | 0.5473  |  0.5473
Frag  |  6  |  -CH2-   [aliphatic carbon]              | 0.4911  |  2.9466
Frag  |  6  |  Aromatic Carbon                        | 0.2940  |  1.7640
Frag  |  1  |  -C(=O)O  [ester, aliphatic attach]      |-0.9505  | -0.9505
Frag  |  1  |  -Hg-  [mercury]                        |-0.7000  | -0.7000
Const |     |  Equation Constant                      |         |  0.2290
-------+-----+-----------------------------------------+---------+--------
Log Kow   =   3.8364
```

MPBPVP (v1.43) Program Results:
==========

Experimental Database Structure Match: no data

SMILES : c1([Hg]OC(=O)CCCCCCC)ccccc1
CHEM   :
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90
---------- SUMMARY MPBVP v1.43 ----------

Boiling Point: 367.78 deg C (Adapted Stein and Brown Method)

Melting Point: 143.13 deg C (Adapted Joback Method)
Melting Point: 101.09 deg C (Gold and Ogle Method)
Mean Melt Pt : 122.11 deg C (Joback; Gold,Ogle Methods)
Selected MP: 115.10 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 367.78 deg C (estimated))
(Using MP: 115.10 deg C (estimated))
VP: 2.34E-006 mm Hg (Antoine Method)
: 0.000312 Pa (Antoine Method)
VP: 6.41E-006 mm Hg (Modified Grain Method)
: 0.000855 Pa (Modified Grain Method)
VP: 1.28E-005 mm Hg (Mackay Method)
: 0.00171 Pa (Mackay Method)
Selected VP: 6.41E-006 mm Hg (Modified Grain Method)
: 0.000855 Pa (Modified Grain Method)
Subcooled liquid VP: 4.98E-005 mm Hg (25 deg C, Mod-Grain method)
: 0.00663 Pa (25 deg C, Mod-Grain method)

```
-------+-----+-------------------+----------+---------
TYPE  | NUM |  BOIL DESCRIPTION  |  COEFF   |  VALUE
-------+-----+-------------------+----------+---------
Group |  1  |  -CH3              |   21.98  |   21.98
Group |  6  |  -CH2-             |   24.22  |  145.32
Group |  1  |  -COO- (ester)     |   78.85  |   78.85
Group |  5  |  CH (aromatic)     |   28.53  |  142.65
```

Group | 1 | -C (aromatic) | 30.76 | 30.76
Group | 1 | Mercury | 130.00 | 130.00
* | | Equation Constant | | 198.18
==========+====================+==========+=========
RESULT-uncorr| BOILING POINT in deg Kelvin | 747.74
RESULT- corr | BOILING POINT in deg Kelvin | 640.94
| BOILING POINT in deg C | 367.78

-------+-----+-------------------+----------+---------
TYPE | NUM | MELT DESCRIPTION | COEFF | VALUE
-------+-----+-------------------+----------+---------
Group | 1 | -CH3 | -5.10 | -5.10
Group | 6 | -CH2- | 11.27 | 67.62
Group | 1 | -COO- (ester) | 53.60 | 53.60
Group | 5 | CH (aromatic) | 8.13 | 40.65
Group | 1 | -C (aromatic) | 37.02 | 37.02
Group | 1 | Mercury | 100.00 | 100.00
* | | Equation Constant | | 122.50
==========+====================+==========+=========
RESULT | MELTING POINT in deg Kelvin | 416.29
| MELTING POINT in deg C | 143.13

Water Sol from Kow (WSKOW v1.41) Results:
==========

Water Sol: 1.201 mg/L

SMILES : c1([Hg]OC(=O)CCCCCCC)ccccc1
CHEM :
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90
---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : 3.84
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 3.84

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s): Value
---------- -----
No Applicable Correction Factors

Log Water Solubility (in moles/L) : -5.544
Water Solubility at 25 deg C (mg/L): 1.201

WATERNT Program (v1.01) Results:
==========

Water Sol (v1.01 est): 0.87295 mg/L

SMILES : c1([Hg]OC(=O)CCCCCCC)ccccc1
CHEM :
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	-0.3213	-0.3213
Frag	6	-CH2- [aliphatic carbon]	-0.5370	-3.2221
Frag	5	Aromatic Carbon (C-H type)	-0.3359	-1.6793
Frag	1	-C(=O)O [ester, aliphatic attach]	0.5757	0.5757
Frag	1	Aromatic Carbon (C-substituent type)	-0.5400	-0.5400
Frag	1	-Hg- [mercury]	-0.7455	-0.7455
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -5.6832
Water Solubility (mg/L) at 25 dec C = 0.87295

HENRYWIN (v3.20) Program Results:
==========

Bond Est : 3.22E-009 atm-m3/mole (3.26E-004 Pa-m3/mole)
Group Est: Incomplete

SMILES : c1([Hg]OC(=O)CCCCCCC)ccccc1
CHEM :
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90

---------- HENRYWIN v3.20 Results ----------

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	15 Hydrogen to Carbon (aliphatic) Bonds		-1.7952
HYDROGEN	5 Hydrogen to Carbon (aromatic) Bonds		-0.7715
FRAGMENT	6 C-C		0.6978
FRAGMENT	1 C-CO		1.7057
FRAGMENT	6 Car-Car		1.5828
FRAGMENT	1 CO-O		0.0714
FRAGMENT	1 Car-Hg	ESTIMATE	0.8900

FRAGMENT | 1 O-Hg | ESTIMATE| 4.5000
---------+---------+---------+---------
RESULT | BOND ESTIMATION METHOD for LWAPC VALUE | TOTAL | 6.881
---------+---------+---------+---------
HENRYs LAW CONSTANT at 25 deg C = 3.22E-009 atm-m3/mole
= 1.31E-007 unitless
= 3.26E-004 Pa-m3/mole

--------+---------+-----------+--------
| GROUP CONTRIBUTION DESCRIPTION | COMMENT | VALUE
--------+---------+-----------+--------
| 1 CH3 (X) | | -0.62
| 5 CH2 (C)(C) | | -0.75
| 1 CH2 (C)(CO) | | -0.15
| 5 Car-H (Car)(Car) | | 0.55
| 1 CO (C)(O) | | 4.09
| MISSING Value for: Car (Car)(Hg)(Car)
| MISSING Value for: UNTYPED(O)(Car)
| MISSING Value for: O (CO)(Hg)
--------+---------+-----------+--------
RESULT | GROUP ESTIMATION METHOD for LOG GAMMA VALUE |
INCOMPLETE | 3.12
--------+---------+-----------+--------

For Henry LC Comparison Purposes:
Exper Database: none available
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 2.956E-006 atm-m3/mole (2.995E-001 Pa-m3/mole)
VP: 6.41E-006 mm Hg (source: MPBPVP)
WS: 1.2 mg/L (source: WSKOWWIN)

Log Octanol-Air (KOAWIN v1.10) Results:
==========

Log Koa: 10.721

SMILES : c1([Hg]OC(=O)CCCCCCC)ccccc1
CHEM :
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90
---------- KOAWIN v1.10 Results ----------

Log Koa (octanol/air) estimate: 10.721
Koa (octanol/air) estimate: 5.255e+010
Using:
Log Kow: 3.84 (KowWin est)

HenryLC: 3.22e-009 atm-m3/mole (HenryWin est)
Log Kaw: -6.881 (air/water part.coef.)

LogKow : ---- (exp database)
LogKow : 3.84 (KowWin estimate)
Henry LC: --- atm-m3/mole(exp database)
Henry LC: 3.22e-009 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate: 10.721 (from KowWin/HenryWin)

AEROWIN Program (v1.00) Results:
==========
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 0.00664 Pa (4.98E-005 mm Hg)
Log Koa (Koawin est): 10.721
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 0.000452
Octanol/air (Koa) model: 0.0129
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 0.0161
Mackay model : 0.0349
Octanol/air (Koa) model: 0.508

AOP Program (v1.92) Results:
==========
SMILES : c1([Hg]OC(=O)CCCCCCC)ccccc1
CHEM :
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90
---------- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) --------
Hydrogen Abstraction = 7.3244 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 1.9498 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 9.2743 E-12 cm3/molecule-sec
HALF-LIFE = 1.153 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 13.840 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches
Fraction sorbed to airborne particulates (phi):

0.0255 (Junge-Pankow, Mackay avg)
0.508 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

BCFBAF Program (v3.00) Results:
==========
SMILES : c1([Hg]OC(=O)CCCCCCC)ccccc1
CHEM :
MOL FOR: C14 H20 O2 Hg1
MOL WT : 420.90
---------- BCFBAF v3.00 ----------
Summary Results:
Log BCF (regression-based estimate): 3.60 (BCF = 3.97e+003 L/kg wet-wt)
Biotransformation Half-Life (days) : 0.194 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 1.87 (BAF = 74.3 L/kg wet-wt)

Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 3.84

Equation Used to Make BCF estimate:
Log BCF = 0.6598 log Kow - 0.333 + Correction

Correction(s): Value
Tin or Mercury compound 1.400

Estimated Log BCF = 3.598 (BCF = 3965 L/kg wet-wt)

==========
Whole Body Primary Biotransformation Rate Estimate for Fish:
==========

TYPE	NUM	LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Linear C4 terminal chain [CCC-CH3]	0.0341	0.0341
Frag	1	Unsubstituted phenyl group (C6H5-)	-0.6032	-0.6032
Frag	5	Aromatic-H	0.2664	1.3319
Frag	1	Methyl [-CH3]	0.2451	0.2451
Frag	6	-CH2- [linear]	0.0242	0.1451
Frag	1	Benzene	-0.4277	-0.4277
L Kow	*	Log Kow = 3.84 (KowWin estimate)	0.3073	1.1791
MolWt	*	Molecular Weight Parameter		-1.0793
Const	*	Equation Constant		-1.5058
RESULT		LOG Bio Half-Life (days)		-0.7120
RESULT		Bio Half-Life (days)		0.1941
NOTE		Bio Half-Life Normalized to 10 g fish at 15 deg C		

==========+==========+==========+==========

Biotransformation Rate Constant:
kM (Rate Constant): 3.571 /day (10 gram fish)
kM (Rate Constant): 2.008 /day (100 gram fish)
kM (Rate Constant): 1.129 /day (1 kg fish)
kM (Rate Constant): 0.6351 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) = 1.871 (BCF = 74.28 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 1.871 (BAF = 74.28 L/kg wet-wt)
Estimated Log BCF (mid trophic) = 1.961 (BCF = 91.42 L/kg wet-wt)
Estimated Log BAF (mid trophic) = 1.961 (BAF = 91.5 L/kg wet-wt)
Estimated Log BCF (lower trophic) = 1.982 (BCF = 95.9 L/kg wet-wt)
Estimated Log BAF (lower trophic) = 1.986 (BAF = 96.75 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = 2.856 (BCF = 717.5 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 3.131 (BAF = 1351 L/kg wet-wt)

Volatilization From Water
==========

Chemical Name:

Molecular Weight : 420.90 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 3.22E-009 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05

HALF-LIFE (hours) :	3.73E+005	4.07E+006
HALF-LIFE (days) :	1.554E+004	1.696E+005
HALF-LIFE (years) :	42.55	464.3

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========
(using 10000 hr Bio P,A,S)

PROPERTIES OF:

Molecular weight (g/mol) 420.9
Aqueous solubility (mg/l) 0
Vapour pressure (Pa) 0
(atm) 0
(mm Hg) 0
Henry 's law constant (Atm-m3/mol) 3.22E-009
Air-water partition coefficient 1.31688E-007
Octanol-water partition coefficient (Kow) 6918.31
Log Kow 3.84
Biomass to water partition coefficient 1384.46
Temperature [deg C] 25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
-Primary tank 0.00 7346.72 10000.00
-Aeration tank 0.00 7346.72 10000.00
-Settling tank 0.00 7346.72 10000.00

STP Overall Chemical Mass Balance:
---
g/h mol/h percent

Influent 1.00E+001 2.4E-002 100.00

Primary sludge 1.32E+000 3.1E-003 13.19
Waste sludge 9.87E-001 2.3E-003 9.87
Primary volatilization 1.37E-006 3.3E-009 0.00
Settling volatilization 3.66E-006 8.7E-009 0.00
Aeration off gas 9.02E-006 2.1E-008 0.00

Primary biodegradation 5.18E-003 1.2E-005 0.05
Settling biodegradation 1.52E-003 3.6E-006 0.02
Aeration biodegradation 2.00E-002 4.7E-005 0.20

Final water effluent 7.67E+000 1.8E-002 76.67

Total removal 2.33E+000 5.5E-003 23.33
Total biodegradation 2.67E-002 6.3E-005 0.27

Level III Fugacity Model (Full-Output):
==========
Chem Name :
Molecular Wt: 420.9
Henry's LC : 3.22e-009 atm-m3/mole (Henrywin program)
Vapor Press : 6.41e-006 mm Hg (Mpbpwin program)
Liquid VP : 4.99e-005 mm Hg (super-cooled)
Melting Pt : 115 deg C (Mpbpwin program)
Log Kow : 3.84 (Kowwin program)
Soil Koc : 2.16e+003 (KOCWIN MCI method)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.0233	27.7	1000
Water	11.5	900	1000
Soil	87.1	1.8e+003	1000
Sediment	1.41	8.1e+003	0

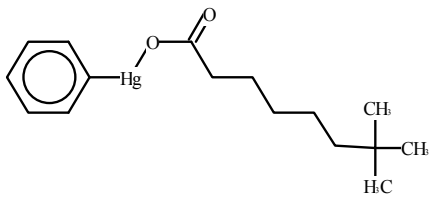
	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	7.26e-013	31.9	12.7	1.06	0.424
Water	2.39e-014	483	628	16.1	20.9
Soil	3.88e-014	1.84e+003	0	61.2	0
Sediment	2.78e-014	6.59	1.54	0.22	0.0513

Persistence Time: 1.83e+003 hr
Reaction Time: 2.32e+003 hr
Advection Time: 8.53e+003 hr
Percent Reacted: 78.6
Percent Advected: 21.4

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 27.67
Water: 900
Soil: 1800
Sediment: 8100
Biowin estimate: 2.589 (weeks-months)

Advection Times (hr):
Air: 100
Water: 1000
Sediment: 5e+004

Phenylmercury neodecanoate



SMILES : c1([Hg]OC(=O)CCCCCC(C)(C)C)ccccc1
CHEM :
MOL FOR: C16 H24 O2 Hg1
MOL WT : 448.96
---------- EPI SUMMARY (v4.00) ----------
Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : ------
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------

KOWWIN Program (v1.67) Results:
==========

Log Kow(version 1.67 estimate): 4.71

SMILES : c1([Hg]OC(=O)CCCCCC(C)(C)C)ccccc1
CHEM :
MOL FOR: C16 H24 O2 Hg1
MOL WT : 448.96

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	-CH3 [aliphatic carbon]	0.5473	1.6419
Frag	5	-CH2- [aliphatic carbon]	0.4911	2.4555
Frag	6	Aromatic Carbon	0.2940	1.7640
Frag	1	-C(=O)O [ester, aliphatic attach]	-0.9505	-0.9505
Frag	1	-tert Carbon [3 or more carbon attach]	0.2676	0.2676
Frag	1	-Hg- [mercury]	-0.7000	-0.7000
Const		Equation Constant		0.2290

Log Kow = 4.7075

MPBPVP (v1.43) Program Results:
==========
Experimental Database Structure Match: no data

SMILES : c1([Hg]OC(=O)CCCCCC(C)(C)C)ccccc1
CHEM   :
MOL FOR: C16 H24 O2 Hg1
MOL WT : 448.96
---------- SUMMARY MPBVP v1.43 ----------

Boiling Point: 379.40 deg C (Adapted Stein and Brown Method)

Melting Point: 168.09 deg C (Adapted Joback Method)
Melting Point: 107.87 deg C (Gold and Ogle Method)
Mean Melt Pt : 137.98 deg C (Joback; Gold,Ogle Methods)
Selected MP: 127.94 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
(Using BP: 379.40 deg C (estimated))
(Using MP: 127.94 deg C (estimated))
VP: 7.47E-007 mm Hg (Antoine Method)
: 9.96E-005 Pa (Antoine Method)
VP: 2.45E-006 mm Hg (Modified Grain Method)
: 0.000327 Pa (Modified Grain Method)
VP: 5.09E-006 mm Hg (Mackay Method)
: 0.000678 Pa (Mackay Method)
Selected VP: 2.45E-006 mm Hg (Modified Grain Method)
: 0.000327 Pa (Modified Grain Method)
Subcooled liquid VP: 2.62E-005 mm Hg (25 deg C, Mod-Grain method)
: 0.00349 Pa (25 deg C, Mod-Grain method)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	3	-CH3	21.98	65.94
Group	5	-CH2-	24.22	121.10
Group	1	>C<	4.50	4.50
Group	1	-COO- (ester)	78.85	78.85
Group	5	CH (aromatic)	28.53	142.65
Group	1	-C (aromatic)	30.76	30.76
Group	1	Mercury	130.00	130.00
*		Equation Constant		198.18
RESULT-uncorr		BOILING POINT in deg Kelvin		771.98
RESULT- corr		BOILING POINT in deg Kelvin		652.56
		BOILING POINT in deg C		379.40

```
-------+-----+-------------------+----------+---------
TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+-------------------+----------+---------
Group |  3  |  -CH3              |   -5.10  |  -15.30
Group |  5  |  -CH2-             |   11.27  |   56.35
Group |  1  |  >C<               |  46.43   |   46.43
Group |  1  |  -COO- (ester)     |  53.60   |   53.60
Group |  5  |  CH (aromatic)     |   8.13   |   40.65
Group |  1  |  -C (aromatic)     |  37.02   |   37.02
Group |  1  |  Mercury           | 100.00   |  100.00
*  |     |  Equation Constant |          |  122.50
============+====================+==========+=========
RESULT    |  MELTING POINT in deg Kelvin  |  441.25
|  MELTING POINT in deg C       |  168.09
-----------------------------------------------------
```

Water Sol from Kow (WSKOW v1.41) Results:
==========

Water Sol: 0.1444 mg/L

SMILES : c1([Hg]OC(=O)CCCCCC(C)(C)C)ccccc1
CHEM :
MOL FOR: C16 H24 O2 Hg1
MOL WT : 448.96
---------- WSKOW v1.41 Results ----------
Log Kow (estimated) : 4.71
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 4.71

Equation Used to Make Water Sol estimate:
Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
(used when Melting Point NOT available)

Correction(s): Value
---------- -----
No Applicable Correction Factors

Log Water Solubility (in moles/L) : -6.493
Water Solubility at 25 deg C (mg/L): 0.1444

WATERNT Program (v1.01) Results:
==========

Water Sol (v1.01 est): 0.19326 mg/L

SMILES : c1([Hg]OC(=O)CCCCCC(C)(C)C)ccccc1
CHEM :
MOL FOR: C16 H24 O2 Hg1
MOL WT : 448.96

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	3	-CH3 [aliphatic carbon]	-0.3213	-0.9638
Frag	5	-CH2- [aliphatic carbon]	-0.5370	-2.6851
Frag	5	Aromatic Carbon (C-H type)	-0.3359	-1.6793
Frag	1	-C(=O)O [ester, aliphatic attach]	0.5757	0.5757
Frag	1	Aromatic Carbon (C-substituent type)	-0.5400	-0.5400
Frag	1	-tert Carbon [3 or more carbon attach]	-0.5774	-0.5774
Frag	1	-Hg- [mercury]	-0.7455	-0.7455
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -6.3661
Water Solubility (mg/L) at 25 dec C = 0.19326

HENRYWIN (v3.20) Program Results:
==========

Bond Est : 5.67E-009 atm-m3/mole (5.74E-004 Pa-m3/mole)
Group Est: Incomplete

SMILES : c1([Hg]OC(=O)CCCCCC(C)(C)C)ccccc1
CHEM :
MOL FOR: C16 H24 O2 Hg1
MOL WT : 448.96

HENRYWIN v3.20 Results

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	19 Hydrogen to Carbon (aliphatic) Bonds		-2.2739
HYDROGEN	5 Hydrogen to Carbon (aromatic) Bonds		-0.7715
FRAGMENT	8 C-C		0.9304
FRAGMENT	1 C-CO		1.7057
FRAGMENT	6 Car-Car		1.5828
FRAGMENT	1 CO-O		0.0714
FRAGMENT	1 Car-Hg	ESTIMATE	0.8900
FRAGMENT	1 O-Hg	ESTIMATE	4.5000
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	6.635

HENRYs LAW CONSTANT at 25 deg C = 5.67E-009 atm-m3/mole

= 2.32E-007 unitless
= 5.74E-004 Pa-m3/mole

GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
3 CH3 (X)		-1.86
4 CH2 (C)(C)		-0.60
1 CH2 (C)(CO)		-0.15
1 C (C)(C)(C)(C)		0.71
5 Car-H (Car)(Car)		0.55
1 CO (C)(O)		4.09
MISSING Value for: Car (Car)(Hg)(Car)		
MISSING Value for: UNTYPED(O)(Car)		
MISSING Value for: O (CO)(Hg)		
RESULT | GROUP ESTIMATION METHOD for LOG GAMMA VALUE |		
INCOMPLETE | 2.74		

For Henry LC Comparison Purposes:
Exper Database: none available
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 1.002E-005 atm-m3/mole (1.016E+000 Pa-m3/mole)
VP: 2.45E-006 mm Hg (source: MPBPVP)
WS: 0.144 mg/L (source: WSKOWWIN)

Log Octanol-Air (KOAWIN v1.10) Results:
==========

Log Koa: 11.345

SMILES : c1([Hg]OC(=O)CCCCCC(C)(C)C)ccccc1
CHEM :
MOL FOR: C16 H24 O2 Hg1
MOL WT : 448.96
---------- KOAWIN v1.10 Results ----------

Log Koa (octanol/air) estimate: 11.345
Koa (octanol/air) estimate: 2.212e+011
Using:
Log Kow: 4.71 (KowWin est)
HenryLC: 5.67e-009 atm-m3/mole (HenryWin est)
Log Kaw: -6.635 (air/water part.coef.)

LogKow : ---- (exp database)

LogKow : 4.71 (KowWin estimate)
Henry LC: --- atm-m3/mole(exp database)
Henry LC: 5.67e-009 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate: 11.345 (from KowWin/HenryWin)

AEROWIN Program (v1.00) Results:
==========
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 0.00349 Pa (2.62E-005 mm Hg)
Log Koa (Koawin est): 11.345
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 0.000859
Octanol/air (Koa) model: 0.0543
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 0.0301
Mackay model : 0.0643
Octanol/air (Koa) model: 0.813

AOP Program (v1.92) Results:
==========
SMILES : c1([Hg]OC(=O)CCCCCC(C)(C)C)ccccc1
CHEM :
MOL FOR: C16 H24 O2 Hg1
MOL WT : 448.96
---------- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) --------
Hydrogen Abstraction = 6.5102 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 1.9498 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 8.4600 E-12 cm3/molecule-sec
HALF-LIFE = 1.264 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 15.172 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
---------- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) ----------

****** NO OZONE REACTION ESTIMATION ******
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database: NO Structure Matches
Fraction sorbed to airborne particulates (phi):
0.0472 (Junge-Pankow, Mackay avg)
0.813 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

HYDROWIN Program (v2.00) Results:
==========
SMILES : c1([Hg]OC(=O)CCCCCC(C)(C)C)ccccc1
CHEM :
MOL FOR: C16 H24 O2 Hg1
MOL WT : 448.96
---------- HYDROWIN v2.00 Results ----------

Currently, this program can NOT estimate a hydrolysis rate constant for
the type of chemical structure entered!!

ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens),
Specific Alkyl Halides & Phosphorus Esters can be estimated!!

When present, various hydrolyzable compound-types will be identified.
For more information, (Click OVERVIEW in Help or see the User's Guide)

***** CALCULATION NOT PERFORMED *****

BCFBAF Program (v3.00) Results:
==========
SMILES : c1([Hg]OC(=O)CCCCCC(C)(C)C)ccccc1
CHEM :
MOL FOR: C16 H24 O2 Hg1
MOL WT : 448.96
---------- BCFBAF v3.00 ----------
Summary Results:
Log BCF (regression-based estimate): 4.17 (BCF = 1.49e+004 L/kg wet-wt)
Biotransformation Half-Life (days) : 0.414 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 2.23 (BAF = 170 L/kg wet-wt)

Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 4.71

Equation Used to Make BCF estimate:
Log BCF = 0.6598 log Kow - 0.333 + Correction

Correction(s): Value
Tin or Mercury compound 1.400

Estimated Log BCF = 4.173 (BCF = 1.489e+004 L/kg wet-wt)

==========

Whole Body Primary Biotransformation Rate Estimate for Fish:

TYPE	NUM	LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	Carbon with 4 single bonds & no hydrogens	-0.2984	-0.2984
Frag	1	Unsubstituted phenyl group (C6H5-)	-0.6032	-0.6032
Frag	5	Aromatic-H	0.2664	1.3319
Frag	3	Methyl [-CH3]	0.2451	0.7353
Frag	5	-CH2- [linear]	0.0242	0.1209
Frag	1	Benzene	-0.4277	-0.4277
L Kow	*	Log Kow = 4.71 (KowWin estimate)	0.3073	1.4468
MolWt	*	Molecular Weight Parameter		-1.1513
Const	*	Equation Constant		-1.5058
RESULT		LOG Bio Half-Life (days)		-0.3827
RESULT		Bio Half-Life (days)		0.4142
NOTE		Bio Half-Life Normalized to 10 g fish at 15 deg C		

Biotransformation Rate Constant:
kM (Rate Constant): 1.673 /day (10 gram fish)
kM (Rate Constant): 0.941 /day (100 gram fish)
kM (Rate Constant): 0.5291 /day (1 kg fish)
kM (Rate Constant): 0.2976 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
Estimated Log BCF (upper trophic) = 2.229 (BCF = 169.5 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 2.229 (BAF = 169.6 L/kg wet-wt)
Estimated Log BCF (mid trophic) = 2.352 (BCF = 224.8 L/kg wet-wt)
Estimated Log BAF (mid trophic) = 2.358 (BAF = 228 L/kg wet-wt)
Estimated Log BCF (lower trophic) = 2.387 (BCF = 243.7 L/kg wet-wt)
Estimated Log BAF (lower trophic) = 2.427 (BAF = 267 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = 3.665 (BCF = 4621 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 4.539 (BAF = 3.457e+004 L/kg wet-wt)

Volatilization From Water

Chemical Name:

Molecular Weight : 448.96 g/mole
Water Solubility : -----
Vapor Pressure : -----
Henry's Law Constant: 5.67E-009 atm-m3/mole (estimated by Bond SAR Method)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05

HALF-LIFE (hours) :	2.188E+005	2.387E+006
HALF-LIFE (days) :	9116	9.946E+004
HALF-LIFE (years) :	24.96	272.3

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
==========
(using 10000 hr Bio P,A,S)
PROPERTIES OF:

Molecular weight (g/mol)	448.96
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry 's law constant (Atm-m3/mol)	5.67E-009
Air-water partition coefficient	2.31886E-007
Octanol-water partition coefficient (Kow)	51286.1
Log Kow	4.71
Biomass to water partition coefficient	10258
Temperature [deg C]	25

Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank	0.00	9535.23	10000.00
-Aeration tank	0.00	9535.23	10000.00
-Settling tank	0.00	9535.23	10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	2.2E-002	100.00
Primary sludge	4.04E+000	9.0E-003	40.37
Waste sludge	2.55E+000	5.7E-003	25.48
Primary volatilization	1.01E-006	2.3E-009	0.00
Settling volatilization	2.50E-006	5.6E-009	0.00
Aeration off gas	6.15E-006	1.4E-008	0.00

Primary biodegradation	1.24E-002	2.8E-005	0.12
Settling biodegradation	3.35E-003	7.5E-006	0.03
Aeration biodegradation	4.41E-002	9.8E-005	0.44
Final water effluent	3.36E+000	7.5E-003	33.56
Total removal	6.64E+000	1.5E-002	66.44
Total biodegradation	5.98E-002	1.3E-004	0.60

Level III Fugacity Model (Full-Output):
==========

Chem Name :
Molecular Wt: 448.96
Henry's LC : 5.67e-009 atm-m3/mole (Henrywin program)
Vapor Press : 2.45e-006 mm Hg (Mpbpwin program)
Liquid VP : 2.55e-005 mm Hg (super-cooled)
Melting Pt : 128 deg C (Mpbpwin program)
Log Kow : 4.71 (Kowwin program)
Soil Koc : 4.7e+003 (KOCWIN MCI method)

Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air 0.0258	30.3	1000
Water 8.62	1.44e+003	1000
Soil 88.4	2.88e+003	1000
Sediment 2.98	1.3e+004	0

Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air 1.16e-012	50.3	22	1.68	0.734
Water 4.61e-014	355	737	11.8	24.6
Soil 4.68e-014	1.82e+003	0	60.6	0
Sediment 7.07e-014	13.6	5.1	0.455	0.17

Persistence Time: 2.85e+003 hr
Reaction Time: 3.82e+003 hr
Advection Time: 1.12e+004 hr
Percent Reacted: 74.5
Percent Advected: 25.5

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 30.34
Water: 1440
Soil: 2880
Sediment: 1.296e+004
Biowin estimate: 2.017 (months)

Advection Times (hr):
Air: 100

Water: 1000
Sediment: 5e+004

Diphenylmercury

CAS Number: 587-85-9
SMILES : [Hg](c(ccc1)cc1)c(ccc2)cc2
CHEM : Diphenyl mercury
MOL FOR: C12 H10 Hg1
MOL WT : 354.80
---------- EPI SUMMARY (v4.00) ----------

Physical Property Inputs:
Log Kow (octanol-water): ------
Boiling Point (deg C) : 204.00
Melting Point (deg C) : ------
Vapor Pressure (mm Hg) : ------
Water Solubility (mg/L): ------
Henry LC (atm-m3/mole) : ------

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.67 estimate) = 3.06

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 332.39 (Adapted Stein & Brown method)
Melting Pt (deg C): 92.55 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 0.0603 (Modified Grain method)
VP (Pa, 25 deg C) : 8.04 (Modified Grain method)
BP (exp database): 204 @ 10 mm Hg deg C
Subcooled liquid VP: 0.271 mm Hg (25 deg C, Mod-Grain method)
: 36.1 Pa (25 deg C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.41):
Water Solubility at 25 deg C (mg/L): 14.2
log Kow used: 3.06 (estimated)
no-melting pt equation used

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 4.1225 mg/L

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 9.68E-006 atm-m3/mole (9.80E-001 Pa-m3/mole)
Group Method: Incomplete
For Henry LC Comparison Purposes:
User-Entered Henry LC: not entered
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 1.982E-003 atm-m3/mole (2.009E+002 Pa-m3/mole)
VP: 0.0603 mm Hg (source: MPBPVP)
WS: 14.2 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:

Log Kow used: 3.06 (KowWin est)
Log Kaw used: -3.403 (HenryWin est)
Log Koa (KOAWIN v1.10 estimate): 6.463
Log Koa (experimental database): None
Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
Vapor pressure (liquid/subcooled): 36.1 Pa (0.271 mm Hg)
Log Koa (Koawin est): 6.463
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 8.3E-008
Octanol/air (Koa) model: 7.13E-007
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 3E-006
Mackay model : 6.64E-006
Octanol/air (Koa) model: 5.7E-005

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 3.8997 E-12 cm3/molecule-sec
Half-Life = 2.743 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 32.913 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
4.82E-006 (Junge-Pankow, Mackay avg)
5.7E-005 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):
Koc : 9161 L/kg (MCI method)
Log Koc: 3.962 (MCI method)
Koc : 452.2 L/kg (Kow method)
Log Koc: 2.655 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.00):
Log BCF from regression-based method = 3.084 (BCF = 1213 L/kg wet-wt)
Log Biotransformation Half-life (HL) = -0.9054 days (HL = 0.1243 days)
Log BCF Arnot-Gobas method (upper trophic) = 1.553 (BCF = 35.77)
Log BAF Arnot-Gobas method (upper trophic) = 1.553 (BAF = 35.77)
log Kow used: 3.06 (estimated)

Volatilization from Water:
Henry LC: 9.68E-006 atm-m3/mole (estimated by Bond SAR Method)
Half-Life from Model River: 115.9 hours (4.827 days)
Half-Life from Model Lake : 1422 hours (59.24 days)

Removal In Wastewater Treatment:
Total removal: 6.73 percent

Total biodegradation: 0.13 percent
Total sludge adsorption: 6.09 percent
Total to Air: 0.52 percent
(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	1.41	65.8	1000
Water	15.3	900	1000
Soil	75.1	1.8e+003	1000
Sediment	8.16	8.1e+003	0

Persistence Time: 1.16e+003 hr

Appendix 3. Toxicity data, terrestrial compartment

Organisms	Toxicological Endpoint	Compound	Dose	Remarks	Reference
B.7.2.1.1 Toxicity soil macroorganisms					
Eisenia fetida	21-day EC50 for the cocoon production	Hg (II)	9,16 mg Hg kg -1 dry weight	Tests were performed as suggested by Van Gestel et al (1989), standardized test conditions	Lock and Janssen, 2001
Eisenia fetida	Significant decrease in regeneration capacity	MeHg (II)	about 5.0 mg kg -1 dry weight	see above	Beyer et al., 1985
Eisenia fetida	21-day NOEC	Hg (II)	10 mg Hg kg -1 dry weight	see above	Lock and Janssen, 2001
Eisenia fetida	21-day LOEC	Hg (II)	18 mg Hg kg -1 dry weight	see above	Lock and Janssen, 2001
Folsomia candida	28-day NOEC	Hg (II)	1,8 mg Hg kg-1 dry weight	Test performed according to the ISO (1999)	Lock and Janssen, 2001
Folsomia candida	28-day LOEL	Hg (II)	3.2 mg Hg kg-1 dry weight	see above	Lock and Janssen, 2001
Folsomia candida	100% mortality	Hg (II)	10 mg Hg kg -1 dry weight	see above	Lock and Janssen, 2001
Folsomia candida	<10% mortality	Hg (II)	5.6 mg Hg kg -1 dry weight	see above	Lock and Janssen, 2001
Folsomia candida	28-day EC50, reproduction	Hg (II)	3.26 mg Hg kg -1 dry weight	see above	Lock and Janssen, 2001
Enchytraeus albidus	42-day EC50, reproduction	Hg (II)	22.0 mg Hg kg -1 dry weight	The test was performed according to OECD Guideline 220	Lock and Janssen, 2001
Enchytraeus albidus	21-day LC50	Hg (II)	26.1 mg Hg kg-1 dry weight	see above	Lock and Janssen, 2001

Organisms	Toxicological Endpoint	Compound	Dose	Remarks	Reference
Enchytraeus albidus	42-day NOEC	Hg (II)	18 mg Hg kg-1 dry weight	see above	Lock and Janssen, 2001
Enchytraeus albidus	42-day LOEC	Hg (II)	32 mg Hg kg-1 dry weight	see above	Lock and Janssen, 2001
Paronychiurus kimi	7-day LC50	Hg (II)	3.9 mg kg-1 dry soil	No well studied laboratory species was used	Son et al., 2007
Paronychiurus kimi	28-day EC50	Hg (II)	0.23 mg kg-1 dry soil	see above	Son et al., 2007
Paronychiurus kimi	Population would head towards extinction	Hg (II)	2.0 mg kg-1 dry soil	see above	Son et al., 2007
Octachaetus pattoni	60-day LD50	Hg (II)	0.79 ppm	No information if the concentration is related to soil dry weight or wet weight, no information on statistical design	Abbasi and Soni, 1983
Octachaetus pattoni	10 day LD50	Hg (II)	2.39 ppm	see above	Abbasi and Soni, 1983
Octachaetus pattoni	10% mortality in 10 days, 35% mortality in 60 days (in controls 0% mortality)	Hg (II)	0.5 ppm (lowest test-conc.)	see above	Abbasi and Soni, 1983
Octachaetus pattoni	100% mortality in 10 days (in controls 0% mortality)	Hg (II)	5.0 ppm (highest test-conc.)	see above	Abbasi and Soni, 1983
Lumbricus terrestris	Average CF of 1.0 for the transfer of Hg from soil to earthworms	Total Hg			Ernst and Frey, 2007
Octolaseon cyaneum	Average CF of 2.3 for transfer of Hg from soil to earthworm	Total Hg			Ernst and Frey, 2007

Organisms	Toxicological Endpoint	Compound	Dose	Remarks	Reference
Lumbricus terrestris	The Phagocyting index decreased significantly	Hg (II)	10-6 M mercury chloride	Coelomocyte test, effects on cellular levels do not indicate any ecological effects	Fugere et al., 1996
Lumbricus terrestris	The Phagocyting index decreased significantly	Hg (II)	10-7 M methylmercury	see above	Fugere et al., 1996
B.7.2.1.2 Toxicity to plants					
Lycopersicon esculentum Mill.	Increased level of endogenous H2O2 at day 10	Hg (II)	50 µM Hg in water	No Guideline but well documented	Cho and Park, 2000
Lycopersicon esculentum Mill.	Accumulation of Hg in roots (1418.9 µg g-1 dry weight at day 20)	Hg (II)	50 µM Hg in water	see above	Cho and Park, 2000
Cucumis sativus L.	Time and concentration-dependet reduction in shoot and root length at day 10 and 15	Hg (II)	Between 0 and 500 µM HgCl2 in medium	Well documented, the seedlings were cultivated in medium containing HgCl2. The effects of the same amounts of mercury in soil could be different because mercury could bind to organic particles.	Cargnelutti et al., 2006
Cucumis sativus L.	Lipid and protein peroxidation increased with increasing mercury concentrations	Hg (II)	Between 0 and 500 µM HgCl2 in medium	see above	Cargnelutti et al., 2006
Cucumis sativus L.	Decreased chlorophyll content	Hg (II)	Between 250 and 500 µM HgCl2 in medium	see above	Cargnelutti et al., 2006

Organisms	Toxicological Endpoint	Compound	Dose	Remarks	Reference
Cucumis sativus L.	Markedly inhibition of catalase activity	Hg (II)	500 µM HgCl2 in medium	see above	Cargnelutti et al., 2006
Pteris vittata	Withering, chlororsis, falling of leaves	Hg (II)	16.7 mg Hg l-1	Well documented but the ferns were obtained from normal stores in the US. The plants could be treated with pesticides before and this could influence the plant's reaction on mercury	Chen et al., 2009
Pteris vittata	H2O2 content in shoots was 290% compared to controls after 7 days	Hg (II)	16.7 mg Hg l-1	see above	Chen et al., 2009
Lupinus termis L.	the transpirationrate of lupines decreased significantly	Phenylmercury acetate	10-5 – 10-3 M phenylmercury acetate in the spraying solution		Ahmed et al., 1987
Pennisetum thyphoideum	Percentage leaf area injured 16.8±1.2; Percentage leaves injured 40±2.2	Hg (II)	10 ppb Hg in nutrient solution for 24 h	Little information about statistical analysis	Mathre and Chaphekar, 1984
B.7.2.1.3 Toxicity to soil microorganisms					
Actinomycetes	Increased population with days after treatment	Ceresan, containing phenylmercury acetate	Application rate of 25,50,75 µg g-1	No Guideline but well documented	Ojo et al., 2007
Fungi	Inhibited population until 48 DAT but started recolonizing the soil right from 63 DAT	Ceresan, containing phenylmercury acetate	Application rate of 25 µg g-1 (below recommended rate of application)	see above	Ojo et al., 2007

Organisms	Toxicological Endpoint	Compound	Dose	Remarks	Reference
Protozoa	Inhibited population	Ceresan, containing phenylmercury acetate	Application rate of 25 µg g-1 (below recommended rate of application)	see above	Ojo et al., 2007
Bacteria	Inhibited population till 33 DAT	Ceresan, containing phenylmercury acetate	Application rate of 25,50,75 µg g-1	see above	Ojo et al., 2007
Bacillus subtilis	DNA damage, using Differential Killing Assay	Phenylmercury acetate	1 mM		Kanematsu et al., 1980
B.7.2.1.4 Toxicity to other terrestrial organisms					
Aiolopus thalassinus	Accumulation factors range from 12.6 to 42.5 in undeveloped eggs after egg pod treatment	Hg (II)	12.1 µg g-1 Hg2+ substrate	Not often used in laboratory studies, Locusta migratoria is a better studied locust	Devkota and Schmidt, 1999
Aiolopus thalassinus	Nymphal duration prolonged	Hg (II)	Fed on food containing 10, 30 and 70 ppm mercury	see above	Schmidt et al., 1992
Aiolopus thalassinus	Fresh body weight of adults was significantly reduced in the F1 generation and the resulting F2 generation	Hg (II)	Fed on food containing 10, 30 and 70 ppm mercury	see above	Schmidt et al., 1992
Aiolopus thalassinus	Weakness in the legs, excited movements of the antennae and legs in addition to tremors in the F1 and also in the F2 adults	Hg (II)	fed on food containing 10, 30 and 70 ppm mercury	see above	Schmidt et al., 1992

Organisms	Toxicological Endpoint	Compound	Dose	Remarks	Reference
Aiolopus thalassinus	1% of the treated animals, the Hg (II)wings became outstretched and bent downwards	Hg (II)	fed on food containing 10, 30 and 70 ppm mercury	see above	Schmidt et al., 1992
Aiolopus thalassinus	Fat body was reduced and the adipose lobes were less numerous than in those of the control	Hg (II)	Fed on food containing 10, 30 and 70 ppm mercury	see above	Schmidt et al., 1992
Drosophila melanogaster	Mutations, Sex-linked Recessive Lethals Assay was used for detection	Ceresan, containing phenylmercury acetate	Adults were fed with nutrients solution containing 20 g Ceresan l-1		Gayathri and Krishnamurthy, 1985
Drosophila melanogaster	Aneuploidy, tested with Non-disjunction Assay	Phenylmercury acetate	Larvae were fed with nutrient solution containing 0.32 mg PMA l-1		Ramel and Magnusson, 1969
B.7.5.1 Toxicity to birds					
Falco sparvinus	All animals died in 39 to 49 days	MeHg	Fed on diet containing 12 ppm MeHg dry weight	Falco sparvinus is no fisheating raptor, naturally it would not feed on an methylmercury rich diet	www.epa.gov,2009
Falco sparvinus	One bird died after 75 days, several individuals showed signs of neurotoxicity after 45 days	MeHg	Fed on diet containing 6 ppm MeHg dry weight	see above	www.epa.gov,2009

Organisms	Toxicological Endpoint	Compound	Dose	Remarks	Reference
Falco sparvinus	No bird died or and no signs of neurotoxicity	MeHg	Fed on diet containing 3 ppm MeHg dry weight	see above	www.epa.gov,2009
Falco sparvinus	Transfer of mercury into eggs, 8.3 ppm wet weight	MeHg	Fed on diet containing 3 ppm MeHg dry weight	Eggs of only one pair were analyzed, small sample size	www.epa.gov,2009
Falco sparvinus	Transfer of mercury into eggs, 18.1 ppm wet weight	MeHg	Fed on diet containing 6 ppm MeHg dry weight	Eggs of only one pair were analyzed, small sample size	www.epa.gov,2009
Falco sparvinus	Transfer of mercury into feathers, 275 ppm in feathers grown during mercury exposure	MeHg	Fed on diet containing 3 ppm MeHg dry weight	Falco sparvinus is no fisheating raptor, naturally it would not feed on an methylmercury rich diet	www.epa.gov,2009
Falco sparvinus	Transfer of mercury into feathers, 542 ppm in feathers grown during mercury exposure	MeHg	Fed on diet containing 6 ppm MeHg dry weight	see above	www.epa.gov,2009
Falco sparvinus	Transfer of mercury into feathers, 542 ppm in feathers grown during mercury exposure	MeHg	Fed on diet containing 6 ppm MeHg dry weight	see above	www.epa.gov,2009
Falco sparvinus	Eggproduction decreased markedly	MeHg	Fed on diet containing 3.3 – 4.6 mg kg-1 MeHg dry weight	see above	www.epa.gov,2009
Falco sparvinus	Nestling fledged reduced, (LOEL)	MeHg	Fed on diet containing 0.7 mg kg-1 MeHg dry weight	see above	www.epa.gov,2009

Organisms	Toxicological Endpoint	Compound	Dose	Remarks	Reference
Falco sparvinus	Total fledging failure at ≥4.6 (EC100)	MeHg	Fed on diet containing 4.6 mg kg-1 MeHg dry weight	see above	www.epa.gov,2009
Anas platyrhynchos	Percentage of eggs outside nestboxes increased, fewer ducklings hatched, small amount of eggshell thinning, ducklins less responsive to tape-recorded maternal call but hyper-responsive to a frightening stimulus in avoidance tests	MeHg	Fed on diet containing 0.5 ppm MeHg	Effects were studied in 3 generations but only one concentration was applied	Heinz, 1979
Tachycineta bicolor	Young females had fewer fledgling than those of the reference site	Total Hg	Mean diet concentration (insects) 0.97±1.11 ppm	Field study; difficult to exclude other influencing factors	Brassso and Cristol 2008
B.7.5.2 Toxicity to mammals					
Blarina brevicauda	38.8 g g-1 mean kidney concentration; mean transfer coefficient of 4.40	Total Hg	Mean diet concentration of 8.82 g g-1		Talmage and Walton, 1993
Rattus norvegicus forma domestica	Dose-dependent increase in testicular lipid peroxidation in response of pro-oxidant exposure; free radical formation increased with increasing dose	Hg(II)	0,50 and 90 ppm HgCl2 in drinking water for 90 days	No information about the daily dose of mercury	Boujbiha et al., 2009

Organisms	Toxicological Endpoint	Compound	Dose	Remarks	Reference
Rattus norvegicus forma domestica (Sprague-Dawley rats)	Significantly more non-viable implantations compared to controls (LOEC)	Hg(II)	1 mg HgCl2 per kg body weight and day for 90 days	Well documented	Heath et al., 2009
Rattus norvegicus forma domestica (Sprague-Dawley rats)	Significantly fewer implantations, more non-viable implantations, lower progesterone, higher levels of luteinizing hormone	Hg(II)	2 mg HgCl2 per kg body weight and day for 90 days	see above	Heath et al., 2009
Mustela vison	All animals died in about a month	MeHg	5 ppm MeHg in diet	Death is a very rough endpoint, the effects of only one concentration were studied, the study provides no information about sublethal concentrations and effects	Aulerich et al., 1974
Mustela vison	No obvious effects, but elevated mercury levels in kidney, that can lead to chronic adverse effects	Hg(II)	10 ppm HgCl2 in diet	Only one mink was analyzed, the effects of only one concentration were studied	Aulerich et al., 1974
Mustela vison	Mercury concentration were related to the presence of the parasite Dictophyma renale	Total Hg		Field study; difficult to exclude confounding factors	Klevanic et al., 2008
Mustela vison	Changes in brain neurochemistry	Total Hg	brain concentrations of 1 mg g-1 wet weight		Basu et al., 2006

Appendix 4. Summary of socio economic impacts

Main economic impacts
The table below summaries the main economic impacts on different actors in the supply chain for phenylmercury substances and interrelated alternatives supply chains.

Table 4.1 Summary of key economic impacts for different actors

	Manufacture of chemicals	Catalyst formulators	Formulators of PU systems (or alternatives)	End-users
Cost of new equipment / facilities or of ceasing use before end of intended life	Phenylmercury compound manufacturers are expected to close their facilities for substance manufacture (though expected to occur under the baseline – i.e. potentially brought forward). Excluding manufacture from the restriction would not reduce cost impacts for EU manufacturers. The loss of export sales is estimated at between€1-4m per year. This may not necessarily be replaced by a mercury free system as their customers may opt to buy mercury compounds from another supplier outside of the EU. There could be an increase in sales for manufacturers of alternative mercury free substances. This is not expected to be significant as 95% of the market is already using mercury free substances.	A possible loss of market but this is not expected to be significant as catalyst formulators will have many other markets within their portfolio.	There will be a one off R&D cost to formulators to switch to a mercury free system (€10-40k per system). Under restriction option 1 (5 year phase out period) the annualised total cost of the restriction is estimated to €0.8-2.49.7m. Under restriction option 2 (2 year phase out period) the annualised total cost is estimated to €0.9-2.614.6m.	Fewer products available on the market. However this could be offset by an increase in mercury free products. There is not expected to be a significant increase in costs as a result of fewer products available on the market.

	Manufacture of chemicals	Catalyst formulators	Formulators of PU systems (or alternatives)	End-users
Changes in operation and maintenance costs (labour, energy, etc.)	Phenylmercury compound manufacturers are expected to close their facilities.	None identified	There is not expected to be any significant changes in operating costs for producing mercury free systems.	There could potentially be increased maintenance costs for products in which PU systems are applied (if performance reduction cannot be resolved - for a small number of uses)
Cost differences between substances (production costs, purchase prices, etc.)	Not relevant	None identified	No expected increase in purchase price of catalysts. It is thought that the small cost of R&D can be passed through to end users.	Increased price of purchasing PU systems (assuming reformulation costs are passed on).
Costs differences due to differences in performance (e.g. efficiency)	Not relevant	None identified		95% of the market uses mercury free compounds
Changes in transportation costs	Not relevant	None identified	None identified	Minimal since 95% of the market uses mercury free compounds

	Manufacture of chemicals	Catalyst formulators	Formulators of PU systems (or alternatives)	End-users
Changes in design, monitoring, training and regulatory costs	Not relevant	Costs of time spent working with users of catalysts (e.g. communications on changes to catalyst products).	There will be a one off R&D cost to formulators of PU systems to switch to a mercury free system (€10-40k per system).	Minimal since 95% of the market uses mercury free compounds

Potential socio economic impacts

The tables below provide the results of an initial review of the types of socio-economic impacts that might be expected in the event of a restriction. This involved identifying various types of socio-economic impacts that were concluded to require further assessment. For each case where it was identified that there was the potential for a significant impact, a summary of the main socio-economic impacts identified (in the preceding analysis) is provided in the following tables.

Table 4.2 Summary of human health impacts

Potential impacts	Restriction option 1	Restriction option 2
Are there any changes in risks to workers health associated with using the substance? (E.g. changes in number being exposed, type of exposure, severity of exposures etc?)	The risk assessment was not focussed on workers health	The risk assessment was not focussed on workers health
Are there any changes in risks to consumer's health associated with using the substance?	Potential improvements to consumer health related to reduced exposure from migration from mercury containing products (e.g. indoor air exposure related to use in flooring).	Potential improvements to consumer health related to reduced exposure from migration from mercury containing products (e.g. indoor air exposure related to use in flooring).
Are there any changes to public health and safety risks?	Potential for reduction of humans exposed via the environment (e.g. through food).	Potential for reduction of humans exposed via the environment (e.g. through food).
Are there any changes in risks to consumer's health associated with known substitutes?	Likely to be of significantly lower risk but relatively little data available on hazards of alternatives.	Likely to be of significantly lower risk but relatively little data available on hazards of alternatives.

Potential impacts	Restriction option 1	Restriction option 2
Are there any changes in risks to workers health associated with using the substance? (E.g. changes in number being exposed, type of exposure, severity of exposures etc?)	The risk assessment was not focussed on workers health	The risk assessment was not focussed on workers health
Are there any significant changes in emissions to air, water, land and/or any significant changes in raw material usage, which could have potential implications for human health?	Only significant change is likely to be in releases of mercury itself (reduction).	Only significant change is likely to be in releases of mercury itself (reduction).

Table 4.3 Summary of environmental impacts

Potential impacts	Restriction option 1	Restriction option 2
Are there any changes in risks for air quality? (e.g. any effect from emissions on acidifying, eutrophication, photochemical or harmful air pollutants that might affect human health, damage crops or buildings or lead to deterioration in the environment (polluted soil or rivers etc)	Expected reduction in risks for various environmental endpoints associated with mercury and methylmercury.	Expected reduction in risks for various environmental endpoints associated with mercury and methylmercury. Reduced impacts could be achieved slightly earlier than under option 1.
Are there any changes in risks to water quality and/or the quantity of water and drinking water?	Should help to reduce concentrations of mercury in water (release via waste water treatment and in particular deposition from air). Also contributes to meeting e.g. objectives under the water framework directive.	Should help to reduce concentrations of mercury in water (release via waste water treatment and in particular deposition from air). Also contributes to meeting e.g. objectives under the water framework directive.
Are there any changes in risks to soil quality and/or the quantity of available soil and usable soil?	Potential reduction in retardation of microbiological activity in soil.	Potential reduction in retardation of microbiological activity in soil.

Potential impacts	Restriction option 1	Restriction option 2
Are there any changes in risks to biodiversity (e.g. the number of species and varieties/races), flora, fauna and/or landscapes (e.g. the scenic value of protected landscape)?	Not known.	Not known.
Are there any changes to waste production (solid, urban, agricultural, industrial, mining, radioactive or toxic waste) or how waste is treated, disposed of or recycled?	No changes expected. Recycling might be an option (in the future) for mercury free alternatives?	No changes expected. Recycling might be an option (in the future) for mercury free alternatives?
Are there any changes in the environmental consequences of firms' activities? (E.g. does this change the use of natural resources required per unit of output and will the process becoming more or less energy intensive? Will this change the operating behaviour of firms to pollute more or less?)	No significant change expected. Equipment for catalyst manufacture, production of polyurethane systems and application methods expected to be the same as with the phenylmercury compounds.	No significant change expected. Equipment for catalyst manufacture, production of polyurethane systems and application methods expected to be the same as with the phenylmercury compounds.
Are there any changes in risks to animal and plant health, food and/or feed safety?	Potential contribution to reduction of mercury concentrations in food, due to reduced environmental concentrations.	Potential contribution to reduction of mercury concentrations in food, due to reduced environmental concentrations.
Are there any significant changes in emissions to air, water, and land or in raw material usage, which could have potential implications for the environment? (e.g. change in raw materials which need to be imported from outside of the EU which leads to additional emissions from transport)	No significant changes expected in emissions of pollutants other than mercury.	No significant changes expected in emissions of pollutants other than mercury.

Table 4.4 Summary of economic impacts

Potential impacts	Restriction option 1	Restriction option 2

Potential impacts	Restriction option 1	Restriction option 2
Are there any changes to operating costs?	There are not expected to any significant operating costs of using alternative Hg free systems. Users may benefit from a reduction in waste disposal costs	There are not expected to any significant operating costs of using alternative Hg free systems Users may benefit from a reduction in waste disposal costs
Are there any changes to investment costs? E.g. costs to avoid risks to human health such as waste and waste water handling.	The annualised cost of compliance over 5 years could be as low as €0.8-2.4m	The annualised cost of compliance over 2 years could be as low as €0.9-2.6m
Are there likely to be changes to profitability? E.g. costs of using an alternative substance can not be passed on along the supply chain.	No – users should be able to switch to a Hg free alternative and continue producing their products. The low costs of compliance may be passed through to higher prices. Loss of profits to manufacturers of these (5) substances is likely to be redistributed to mercury free alternatives It is also possible that some manufacturers also produce mercury free alternatives within their portfolio and therefore there may also just be redistribution internally of production and resources.	No – users should be able to switch to a Hg free alternative and continue producing their products. The low costs of compliance may be passed through to higher prices. Loss of profits to manufacturers of these (5) substances is likely to be redistributed to mercury free alternatives It is also possible that some manufacturers also produce mercury free alternatives within their portfolio and therefore there may also just be redistribution internally of production and resources.

Potential impacts	Restriction option 1	Restriction option 2
Are there likely to be changes to sales and turnover? E.g. a loss of functionality leads to reduction in demand	No – users should be able to switch to a Hg free alternative and continue producing their products. Loss of sales to manufacturers of these (5) substances is likely to be redistributed to increased sales in mercury free alternatives It is also possible that some manufacturers also produce mercury free alternatives within their portfolio and therefore there may also just be redistribution internally of production and resources.	No – users should be able to switch to a Hg free alternative and continue producing their products. Loss of sales to manufacturers of these (5) substances is likely to be redistributed to increased sales in mercury free alternatives It is also possible that some manufacturers also produce mercury free alternatives within their portfolio and therefore there may also just be redistribution internally of production and resources.
Are there likely to be changes to administration costs?	Users will initially incur some search costs associated with finding a suitable alternative and "menu" costs from trying to find a cheap and reliable supplier. This is unlikely to be significant.	Users will initially incur some search costs associated with finding a suitable alternative and "menu" costs from trying to find a cheap and reliable supplier. This is unlikely to be significant.
Are there likely to be changes to innovation and research?	Industry with MCPUE systems will need to invest in R&D time and resources to find a suitable mercury free alternatives	Industry with MCPUE systems will need to invest in R&D time and resources to find a suitable mercury free alternatives
Are there likely to be changes to the market price?	Given the low costs of compliance and that the costs of Hg free alternatives are expected to be similar there is unlikely to be any significant increases in prices.	Given the low costs of compliance and that the costs of Hg free alternatives are expected to be similar there is unlikely to be any significant increases in prices.
Are there likely to be changes to the quality of the final product?	There are not expected to be any loss of functionality to end uses where there is a Hg free alternative. The 5 year time period is anticipated to be sufficient to replace virtually all current MCPUE systems.	There are not expected to be any loss of functionality to end uses where there is a Hg free alternative. The shorter 2 year phase out time scale could be problematic for some uses where it is expected that it will be difficult to find and develop a suitable Hg free alternative.

Potential impacts	Restriction option 1	Restriction option 2
Are there likely to be changes to employment?	No – users should be able to switch to a Hg free alternative and continue producing their products. Loss of employment to manufacturers of these (5) substances is likely to be redistributed by increased employed in mercury free alternatives. It is also possible that some manufacturers also produce mercury free alternatives within their portfolio and therefore there may also just be redistribution internally of production and resources.	No – users should be able to switch to a Hg free alternative and continue producing their products. Loss of employment to manufacturers of these (5) substances is likely to be redistributed by increased employed in mercury free alternatives. It is also possible that some manufacturers also produce mercury free alternatives within their portfolio and therefore there may also just be redistribution internally of production and resources.
Are there likely to be changes to monitoring, compliance and enforcement?	There will be some additional costs to competent authorities to check imports of substances and ensuring there is no use or production of these substances in the EU	There will be some additional costs to competent authorities to check imports of substances and ensuring there is no use or production of these substances in the EU
Are there likely to be changes to the trend in sales and production?	Sales revenue is likely to be redistributed to mercury free alternatives rather than any loss of output at an EU level in case the proposed restrictions cover imported articles as well	Sales revenue is likely to be redistributed to mercury free alternatives rather than any loss of output at an EU level in case the proposed restrictions cover imported articles as well
Are there likely to be changes to the cost associated with substitutes?	Given the low costs of compliance and that the costs of Hg free alternatives are expected to be similar there is unlikely to be any significant price changes for Hg free alternatives.	Given the low costs of compliance and that the costs of Hg free alternatives are expected to be similar there is unlikely to be any significant price changes for Hg free alternatives.
Are there likely to be changes to the performance and product quality associated with substitutes?	There are not expected to be any loss of functionality to end uses where there is a Hg free alternative	There are not expected to be any loss of functionality to end uses where there is a Hg free alternative

Potential impacts	Restriction option 1	Restriction option 2
Are there likely to be any changes in the process used that may have an impact on economic costs?	No - machinery and equipment used for mercury free systems is virtually the same as that used by MCPUE systems	No - machinery and equipment used for mercury free systems is virtually the same as that used by MCPUE systems
Are there likely to be any changes in emissions to air, water, land and/or any changes in raw material usage, which could have potential economic costs?	Users may benefit from a reduction in waste disposal costs	Users may benefit from a reduction in waste disposal costs

Table 4.5 Summary of social impacts

Potential impacts	Restriction option 1	Restriction option 2
Are there any likely to be changes in employment at an EU level?	There may be some job losses for manufacturers that predominately export these mercury compounds. Likely to be mostly a redistribution of jobs to producers of mercury free alternatives or simply changes in production to produce mercury free alternatives.	There may be some job losses for manufacturers that predominately export these mercury compounds. Likely to be mostly a redistribution of jobs to producers of mercury free alternatives or simply changes in production to produce mercury free alternatives.
Are there any likely to be changes in employment at a MS level?	Likely to be mostly a redistribution of jobs to producers of mercury free alternatives	Likely to be mostly a redistribution of jobs to producers of mercury free alternatives
Are there any likely to be changes in employment outside of the EU?	Since the restriction includes the restriction on imported articles there is unlikely to be a significant change in employment although some additional employment might occur to replace EU exports.	Since the restriction includes the restriction on imported articles there is unlikely to be a significant change in employment although some additional employment might occur to replace EU exports.

Table 4.6 Summary of competition, trade and wider economic impacts

Potential impacts	Restriction option 1	Restriction option 2

Potential impacts	Restriction option 1	Restriction option 2
Are there any likely to be changes to competition within the EU? (e.g. changes in the number of products available to downstream users and consumers)	Given the market is heavily dominated already by mercury free catalysts there is not expected to be a significant macro-economic impact. The restriction will give a competitive advantage to companies producing and using mercury free catalysts.	Given the market is heavily dominated already by mercury free catalysts there is not expected to be a significant macro-economic impact. The restriction will give a competitive advantage to companies producing and using mercury free catalysts.
Are there any likely to be changes to competitiveness outside of the EU? (E.g. would the conditions of the restriction give an advantage to manufacturers outside of the EU?)	No - since the restriction includes the restriction on imported articles.	No - since the restriction includes the restriction on imported articles.
Are there any likely to be changes to international trade? (e.g. trade flows between EU and non-EU countries)	Export and import volumes of the compounds themselves are fairly insignificant from at an EU trade volume perspective. However the impacts on imported articles may be more significant.	Export and import volumes of the compounds themselves are fairly insignificant from at an EU trade volume perspective. However the impacts on imported articles may be more significant.
Are there any likely to be changes in investment flows? (e.g. businesses deciding to locate outside of the EU)	There might be an increase in investment and trade flows over time for mercury free EU producers and products if there is a global effort to remove these mercury compounds.	No - since the restriction includes the restriction on imported articles. There might be an increase in investment and trade flows over time for mercury free EU producers and products if there is a global effort to remove these mercury compounds.

Appendix 5. Assumptions regarding use and releases

Introduction
In the analysis presented in this report, the quantities of phenylmercury compounds used and the amounts released to the environment are a key factor in determining the scale of:
-likely reductions in emissions to the environment that could be achieved through a restriction; and
-potential costs of replacing these compounds with alternatives.

This appendix provides details of the assumptions used in estimating future usage and release of the substances as a basis for various other calculations used in the analysis.
All figures are presented in tonnes.

'Current' manufacture, trade and use
Data for 2007 are included in Section B in terms of production, import, export and use in the EU of the five phenylmercury compounds. These are reproduced below.

	Phenylmercury acetate	Phenylmercury propionate	Phenylmercury 2-ethylhexanoate	Phenylmercuric octanoate	Phenylmercury neodecanoate
Production	5-10	~ 0	50-100	~ 0	75-150
Export	5-10	~ 0	49-99	~ 0	40 - 85
Import	<1	~ 0	~ 0	~ 0	< 5
For use in EU+EFTA	<1	~ 0	< 1	~ 0	36 - 70

Predicting future use of the substances
It is understood that use of the mercury compounds 10 years ago was 2-3 times greater than current levels.

The consultation undertaken for the current analysis (see Section B.2, C and F), indicates that there are significant ongoing efforts and pressures to further replace mercury-based catalysts in polyurethane products. However, no comprehensive data are available on the likely pace of future decline in use of the substances.

Whilst there is significant uncertainty in the rate of decline, it seems clear that there will continue to be a decline in use. However, it also seems clear that there are some uses of these compounds that will require additional time and effort if their replacement is to be achieved. Therefore, it is unlikely that these substances will be fully replaced by alternatives in the short to medium term without any additional regulatory pressure.

As such, for the purposes of this analysis, it has been assumed that use will continue to decline in the coming years but that use will not decline to zero over the timeframe of the analysis. The decline in use is therefore assumed to follow an exponential path, based on the historical decline.

Taking phenylmercury neodecanoate as an example, use in 2007 was estimated at 36-70 tonnes. Assuming that use 10 years previously was 2.5 times greater (i.e. the midpoint of 2 to 3 times greater), this corresponds to 90-175 tonnes. Therefore, the use profile over the assessment timescale – up to 2030 – is assumed to be as follows.

Year	Emissions (tonnes)	
	High	Low
1997	175	90
1998	160	82
1999	146	75
2000	133	68
2001	121	62
2002	111	57
2003	101	52
2004	92	47
2005	84	43
2006	77	39
2007	70	36
2008	64	33
2009	58	30
2010	53	27
2011	49	25
2012	44	23
2013	40	21
2014	37	19
2015	34	17
2016	31	16
2017	28	14
2018	26	13
2019	23	12
2020	21	11
2021	19	10
2022	18	9
2023	16	8
2024	15	8
2025	13	7
2026	12	6
2027	11	6
2028	10	5
2029	9	5
2030	9	4

Using these assumptions, therefore, use in 2007 was 40% of use in 1997. Similarly, use in 2017 is assumed to be 40% of use in 2007 and use in 2020 is assumed to be around 30% of use in 2007.

Applying this approach to the manufacture and usage figures for all of the compounds, the following figures have been used as estimates for 2020, corresponding to the figures above for 2007.

	Phenylmercury acetate	Phenylmercury propionate	Phenylmercury 2-ethylhexanoate	Phenylmercuric octanoate	Phenylmercury neodecanoate
Production	2-3	~ 0	15-30	~ 0	23-46
Export	2-3	~ 0	15-30	~ 0	12-26
Import	<1	~ 0	~ 0	~ 0	< 5
For use in EU+EFTA	<1	~ 0	< 1	~ 0	12-26

Since production and use of the propionate and octanoate compounds appear to be negligible, the focus is on the remaining three compounds. Phenylmercury neodecanoate is understood to be the only compound used to any significant degree in the EU. Phenylmercury acetate and 2-ethylhexanoate are produced in the EU but exported to outside the EU; they have therefore been considered together.

Based on this approach, key data on production and use for the compounds of most interest are set out below. It is assumed that production/use is at the upper end of the range quoted, for consistency with the release and exposure assessment in Section B.

	Emissions (tonnes)	
	Neodecanoate	Acetate and 2-EHA
Produced in 2007	150	110
Produced in 2030	18	13.4
Cumulative production 2015-2030	633	464
Cumulative production 2018-2030	435	319
Cumulative production 20011-30	997	731
Used in 2007	70	<1
Used in 2010	9	<1
Cumulative use 2015-2030	295	<1
Cumulative use 2018-2030	203	<1
Cumulative use 2011-30	465	<1

Estimates of releases to the environment

Section B of this dossier provides estimates of releases of the mercury compounds to the environment, based on current production and use levels (data relate to 2008). This is reproduced below.

Table from Part B.9 (tonnes Hg/year) (2008 data)

Life cycle stage	Air	Waste water	Landfills
Manufacturing	<0.0003	0.0002	n.d.
Formulation and processing	2.4	0.01	0.003
Service life	2.9	0.3	18.4
Waste incineration	0.8	0.001	6.6
Landfilling	0.3	-	-
Total emission	6.3	0.3	25

For the purposes of providing an indicative estimate of the likely future releases to the environment that could be avoided through a restriction under option 1 (restriction from 2018), the following approach has been taken:

It is assumed that use of the substances will decline in line with the estimates provided above.

It is assumed that releases to air and waste water are the most critical as regards exposure and potential for environmental harm. Releases to landfill are only relevant when subsequently released to other environmental media (except in the context of potential controls on hazardous waste disposal) and so the right hand column in the table above is not included in the subsequent analysis.

It is assumed that environmental releases change in proportion to use.

It is assumed that the average product lifetime is 5 years. Whilst it is recognised that several products may have longer lifetimes than this (e.g. flooring is assumed to be 10 years in the exposure assessment, several of the product types detailed earlier in the assessment are likely to have much shorter timescales and thus 5 years is assumed to be reasonable).

Emissions from manufacturing are not included in this analysis because they are considered to be negligible based on the above.

For emissions from formulation and processing, emissions are assumed to occur in the year in which use takes place. Emissions in 2018, therefore, are based on the proportion of use in 2008 (0.40) multiplied by the annual emission in 2008 (2.41t) to give emissions of 0.96t. Emissions in subsequent years are calculated based on use of a factor proportional to the use in the year in question.

For service life emissions, emissions in 2018 are assumed to be based on the releases from those products that enter into use in that year. This is based on the 'steady state' emission estimate for 2008 (3.2t), multiplied by the proportion of 2008 use in 2018 (0.40), multiplied by 1/5 to take into account that the 2008 emissions are based on a steady state and assuming that the 5 year lifetime applies, giving emissions of 0.26t. Likewise, emissions in 2019 are then based on the second year's emissions from products entering into use in 2018 (0.26t) plus emissions from products entering into use in 2019, which is again based on the 2008

emissions (3.2t), multiplied by the proportion of 2008 use in 2019 (0.36) and by 1/5, giving 0.23t + 0.26t = 0.49t. This process is continued for subsequent years, with emissions in each year comprised of releases from products entering into use over the preceding 5 years. For emissions in 2018 to 2021, releases from products entering into use prior to 2018 are not included because they would not be directly affected by the restriction.

Emissions from waste incineration are based on the emissions in 2008 (0.80t) multiplied by the fraction of 2008 usage. It is assumed that products will not enter the waste phase and hence be incinerated for five years (the assumed product lifetime), such that emissions in 2023 are based on the fraction of 2008 use that occurs in 2018 (0.40) multiplied by 0.80t, to give 0.32t.

Emissions from landfills in 2008 are, in the exposure assessment, calculated to be 0.3t over a period of 20 years. Therefore, if a steady state were to apply, annual emissions would be 0.3t, relating to products land filled over the previous 20 years (i.e. 0.015t for the quantities land filled in each year). This is based on an emission factor of 0.05% and the amount assumed to be disposed of to landfill (27t).

For the purposes of this analysis, emissions from landfills are assumed to occur with a 5 year lag due to the assumed service life of the products. Thus, products entering into use in 2018 will be land filled in 2023. So, emissions in 2023 are 1/20 of those related to use in 2018 (which is 0.40 as a fraction of 2008 use), i.e. 0.40 multiplied by 0.3t as the 2008 steady state value multiplied by 1/20 = 0.006t. Then, in 2024, emissions are 2/10 of those related to use in 2018 (0.006t) plus the same for use in 2019 (0.36 x 0.4t x 1/20 = 0.0055t), giving a total of 0.011t. Emissions related to use in years prior to the restriction (2018) are not included because they would not be affected by the proposed restriction.

Appendix 6. EUSES Phenylmercury acetate

EUSES 2.1.1 10-06-2010 09:37:28

EUSES 2 Compact report	Single substance
Printed on	10-06-2010 09:37:28
Study	phenylmercury acetate C
Substance	Phenylmercury acetate
Defaults	Standard Euses 2.1
Assessment types	1B, 2, 3B
Base set complete	No
Explanation status column	O = Output; D = Default; S = Set; I = Imported

Name	Value	Units	Status
STUDY			
STUDY IDENTIFICATION			
Study name	phenylmercury acetate C		S
Study description	phenylmercury acetate C		S
Author	Thomas Hartnik		D
Institute	Climate and Pollution directorate		S
Address			D
Zip code			D
City	Oslo		S
Country	Norway		S
Telephone			D
Telefax			D
Email			D
Calculations checksum	D7AA9AE0		S

EUSES 2 Compact report	Single substance
Printed on	10-06-2010 09:37:28
Study	phenylmercury acetate C
Substance	Phenylmercury acetate
Defaults	Standard Euses 2.1
Assessment types	1B, 2, 3B
Base set complete	No

Explanation status column O = Output; D = Default; S = Set; I = Imported

Name	Value	Units	Status
DEFAULTS			
RELEASE ESTIMATION			
Fraction of EU production volume for region	1	[%]	S

EUSES 2 Compact report	Single substance
Printed on	10-06-2010 09:37:28
Study	phenylmercury acetate C
Substance	Phenylmercury acetate
Defaults	Standard Euses 2.1
Assessment types	1B, 2, 3B
Base set complete	No

Explanation status column O = Output; D = Default; S = Set; I = Imported

Name	Value	Units	Status
SUBSTANCE			
SUBSTANCE IDENTIFICATION			
General name	Phenylmercury acetate		S
Description			D
CAS-No	62-38-4		S
EC-notification no.			D
EINECS no.	200-532-5		S
PHYSICO-CHEMICAL PROPERTIES			
Molecular weight	336.75	[g.mol-1]	S
Melting point	150	[oC]	S
Boiling point	??	[oC]	D
Vapour pressure at test temperature	6E-06	[mmHg]	S
Temperature at which vapour pressure was measured	20	[oC]	S
Vapour pressure at 25 [oC]	1.13E-03	[Pa]	O
Octanol-water partition coefficient	0.71	[log10]	S
Water solubility at test temperature	4.37E+03	[mg.l-1]	S
Temperature at which solubility was measured	15	[oC]	S
Water solubility at 25 [oC]	5.03E+03	[mg.l-1]	O
PARTITION COEFFICIENTS AND BIOCONCENTRATION FACTORS			
SOLIDS-WATER			
Chemical class for Koc-QSAR	Esters		S
Organic carbon-water partition coefficient	8.3E+03	[l.kg-1]	S
BIOCONCENTRATION FACTORS			
PREDATOR EXPOSURE			
Bioconcentration factor for earthworms	100	[l.kgwwt-1]	S
HUMAN AND PREDATOR EXPOSURE			
Biomagnification factor in fish	2.5	[-]	S
BIOTA-WATER			
FOR REGIONAL/CONTINENTAL DISTRIBUTION			
Bioconcentration factor for aquatic biota	100	[l.kgwwt-1]	S

EUSES 2 Compact report	Single substance
Printed on	10-06-2010 09:37:28
Study	phenylmercury acetate C
Substance	Phenylmercury acetate
Defaults	Standard Euses 2.1
Assessment types	1B, 2, 3B
Base set complete	No

Explanation status column: O = Output; D = Default; S = Set; I = Imported

Name	Value	Units	Status
RELEASE ESTIMATION			
CHARACTERIZATION AND TONNAGE			
Production volume of chemical in EU	120	[tonnes.yr-1]	S
Fraction of EU production volume for region	1	[%]	S
Volume of chemical imported to EU	3	[tonnes.yr-1]	S
Volume of chemical exported from EU	90	[tonnes.yr-1]	S
USE PATTERNS			
PRODUCTION STEPS			
EMISSION INPUT DATA			
Industry category	11 Polymers industry		S
Use category	55/0 Others		S
Extra details on use category	Polymerization processes		S
Extra details on use category	Wet: catalysts		S
Main category production	III Multi-purpose equipment		S
Emission scenario	no special scenario selected/available		S
INTERMEDIATE RESULTS			
INTERMEDIATE			
RELEASE FRACTIONS AND EMISSION DAYS			
PRODUCTION			
Emission tables	A1.1 (general table), B1.9 (specific uses)		S
RELEASE FRACTIONS			
Fraction of tonnage released to air	0.0525	[-]	S
Fraction of tonnage released to wastewater	2.5E-03	[-]	S
EMISSION DAYS			
Fraction of the main local source	0.01	[-]	S
Number of emission days per year	300	[-]	S

EUSES 2 Compact report	Single substance
Printed on	10-06-2010 09:37:28
Study	phenylmercury acetate C
Substance	Phenylmercury acetate
Defaults	Standard Euses 2.1
Assessment types	1B, 2, 3B
Base set complete	No

Explanation status column O = Output; D = Default; S = Set; I = Imported

Name	Value	Units	Status
DISTRIBUTION			
REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	2.78E-06	[mg.l-1]	O
Regional PEC in seawater (total)	3.06E-07	[mg.l-1]	O
Regional PEC in surface water (dissolved)	2.75E-06	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	3.04E-07	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	3.42E-11	[mg.m-3]	O
Regional PEC in agricultural soil (total)	6.34E-04	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	4.32E-06	[mg.l-1]	O
Regional PEC in natural soil (total)	6.31E-04	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	6.43E-04	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	9.26E-04	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	9.27E-05	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	2.36E-06	[mg.l-1]	O
Continental PEC in seawater (total)	3.92E-08	[mg.l-1]	O
Continental PEC in surface water (dissolved)	2.34E-06	[mg.l-1]	O
Continental PEC in seawater (dissolved)	3.9E-08	[mg.l-1]	O
Continental PEC in air (total)	1.96E-11	[mg.m-3]	O
Continental PEC in agricultural soil (total)	3.74E-04	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	2.55E-06	[mg.l-1]	O
Continental PEC in natural soil (total)	3.61E-04	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	3.75E-04	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	7.87E-04	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	1.19E-05	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	3.26E-08	[mg.l-1]	O
Moderate PEC in water (dissolved)	3.25E-08	[mg.l-1]	O
Moderate PEC in air (total)	2.14E-15	[mg.m-3]	O
Moderate PEC in soil (total)	3.95E-08	[mg.kgwwt-1]	O

Moderate PEC in sediment (total)	9.89E-06	[mg.kgwwt-1]	O

GLOBAL: ARCTIC

Arctic PEC in water (total)	3.26E-08	[mg.l-1]	O
Arctic PEC in water (dissolved)	3.24E-08	[mg.l-1]	O
Arctic PEC in air (total)	1.38E-16	[mg.m-3]	O
Arctic PEC in soil (total)	9.23E-09	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	9.88E-06	[mg.kgwwt-1]	O

GLOBAL: TROPIC

Tropic PEC in water (total)	3.13E-08	[mg.l-1]	O
Tropic PEC in water (dissolved)	3.11E-08	[mg.l-1]	O
Tropic PEC in air (total)	1.67E-15	[mg.m-3]	O
Tropic PEC in soil (total)	1.55E-08	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	9.48E-06	[mg.kgwwt-1]	O

EUSES 2 Compact report	Single substance
Printed on	10-06-2010 09:37:28
Study	phenylmercury acetate C
Substance	Phenylmercury acetate
Defaults	Standard Euses 2.1
Assessment types	1B, 2, 3B
Base set complete	No

Explanation status column O = Output; D = Default; S = Set; I = Imported

Name	Value	Units	Status
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	1.89E-04	[%]	O
Steady-state mass fraction in regional seawater	2.31E-05	[%]	O
Steady-state mass fraction in regional air	2.61E-08	[%]	O
Steady-state mass fraction in regional agricultural soil	0.0978	[%]	O
Steady-state mass fraction in regional natural soil	0.0109	[%]	O
Steady-state mass fraction in regional industrial soil	4.13E-03	[%]	O
Steady-state mass fraction in regional freshwater sediment	7.25E-04	[%]	O
Steady-state mass fraction in regional seawater sediment	2.42E-05	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	0.0141	[%]	O
Steady-state mass fraction in continental seawater	0.518	[%]	O
Steady-state mass fraction in continental air	2.59E-06	[%]	O
Steady-state mass fraction in continental agricultural soil	5.05	[%]	O
Steady-state mass fraction in continental natural soil	0.549	[%]	O
Steady-state mass fraction in continental industrial soil	0.211	[%]	O
Steady-state mass fraction in continental freshwater sediment	0.0539	[%]	O
Steady-state mass fraction in continental seawater sediment	0.0271	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	24	[%]	O
Steady-state mass fraction in moderate air	3.15E-09	[%]	O
Steady-state mass fraction in moderate soil	2.47E-03	[%]	O
Steady-state mass fraction in moderate sediment	0.251	[%]	O
GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	15.7	[%]	O
Steady-state mass fraction in arctic air	1.11E-10	[%]	O
Steady-state mass fraction in arctic soil	2.52E-04	[%]	O
Steady-state mass fraction in arctic sediment	0.164	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	52.8	[%]	O
Steady-state mass fraction in tropic air	4.02E-09	[%]	O

Steady-state mass fraction in tropic soil	9.55E-04	[%]	O
Steady-state mass fraction in tropic sediment	0.552	[%]	O

EUSES 2 Compact report	Single substance
Printed on	10-06-2010 09:37:28
Study	phenylmercury acetate C
Substance	Phenylmercury acetate
Defaults	Standard Euses 2.1
Assessment types	1B, 2, 3B
Base set complete	No

Explanation status column O = Output; D = Default; S = Set; I = Imported

Name Value Units Status

STEADY-STATE MASSES

REGIONAL

Steady-state mass in regional freshwater	10	[kg]	O
Steady-state mass in regional seawater	1.22	[kg]	O
Steady-state mass in regional air	1.38E-03	[kg]	O
Steady-state mass in regional agricultural soil	5.17E+03	[kg]	O
Steady-state mass in regional natural soil	579	[kg]	O
Steady-state mass in regional industrial soil	219	[kg]	O
Steady-state mass in regional freshwater sediment	38.4	[kg]	O
Steady-state mass in regional seawater sediment	1.28	[kg]	O

CONTINENTAL

Steady-state mass in continental freshwater	745	[kg]	O
Steady-state mass in continental seawater	2.74E+04	[kg]	O
Steady-state mass in continental air	0.137	[kg]	O
Steady-state mass in continental agricultural soil	2.67E+05	[kg]	O
Steady-state mass in continental natural soil	2.9E+04	[kg]	O
Steady-state mass in continental industrial soil	1.12E+04	[kg]	O
Steady-state mass in continental freshwater sediment	2.85E+03	[kg]	O
Steady-state mass in continental seawater sediment	1.43E+03	[kg]	O

GLOBAL: MODERATE

Steady-state mass in moderate water	1.27E+06	[kg]	O
Steady-state mass in moderate air	1.67E-04	[kg]	O
Steady-state mass in moderate soil	131	[kg]	O
Steady-state mass in moderate sediment	1.33E+04	[kg]	O

GLOBAL: ARCTIC

Steady-state mass in arctic water	8.31E+05	[kg]	O
Steady-state mass in arctic air	5.87E-06	[kg]	O
Steady-state mass in arctic soil	13.3	[kg]	O
Steady-state mass in arctic sediment	8.69E+03	[kg]	O

GLOBAL: TROPIC

Steady-state mass in tropic water	2.79E+06	[kg]	O

Steady-state mass in tropic air	2.13E-04	[kg]	O
Steady-state mass in tropic soil	50.5	[kg]	O
Steady-state mass in tropic sediment	2.92E+04	[kg]	O

EUSES 2 Compact report	Single substance
Printed on	10-06-2010 09:37:28
Study	phenylmercury acetate C
Substance	Phenylmercury acetate
Defaults	Standard Euses 2.1
Assessment types	1B, 2, 3B
Base set complete	No

Explanation status column O = Output; D = Default; S = Set; I = Imported

Name	Value	Units	Status
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	4.8E-07	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	5.27E-06	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in surface water (dissolved)	4.82E-06	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	9.55E-04	[mg.kgwwt-1]	O
Local PEC in seawater during emission episode (dissolved)	7.98E-07	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	7.1E-07	[mg.l-1]	O
Local PEC in marine sediment during emission episode	1.45E-04	[mg.kgwwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	1.54E-03	[mg.kgwwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	1.54E-03	[mg.kgwwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1E-03	[mg.kgwwt-1]	O
Local PEC in pore water of agricultural soil	1.05E-05	[mg.l-1]	O
Local PEC in pore water of grassland	6.85E-06	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	1.05E-05	[mg.l-1]	O

Appendix 7. Classification in Annex I of Directive 67/548/EEC and in Annex VI of Regulation (EC) No 1272/2008 (CLP Regulation)

<table>
<tr><td colspan="3">Phenylmercury acetate
CAS No. 62-38-4
EINECS No. 200-532-5
EINECS Name Phenylmercury acetate
Included in index 080-004-00-5</td></tr>
<tr><td rowspan="2">Classification according to Annex IV of the Regulation (EC) 790/200932</td><td colspan="2">Classification and labelling according to CLP Regulation, 1st ATP from Annex I of the Regulation (EC) 790/2009</td></tr>
<tr><td>Hazard Class and Category Code(s)</td><td>Hazard statement Code(s)</td></tr>
<tr><td>T;R25-48/24/25
C;R34
N;R50/53</td><td>Acute Tox. 3*: Acute toxicity (oral) , hazard category 3 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation)
Skin Corr. 1B: Skin corrosion/irritation, hazard category 1B
STOT RE 1: Specific target organ toxicity – repeated exposure, hazard category 1
Aquatic Acute 1: Hazardous to the aquatic environment, acute hazard category 1
Aquatic Chronic 1: Hazardous to the aquatic environment, chronic hazard category 1</td><td>H301: Toxic if swallowed
H314: Causes severe skin burns and eye damage
H372**: Causes damage to organs (state all organs affected, if known) through prolonged or repeated exposure (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard) (** meaning Route of exposure cannot be excluded, see Annex VI, chapter 1.2.2 of the CLP Regulation)
H400: Very toxic to aquatic life
H410: Very toxic to aquatic life with long lasting effects</td></tr>
</table>

32 Amending the Table 3.2 List of harmonised classification and labelling of hazardous substances from Annex I to Directive 67//548/EEC, 31st ATP

Phenylmercury propionate CAS No. 103-27-5 EINECS No. 203-094-3 EINECS Name Phenylmercury propionate Included in index 080-004-00-7 “organic compounds of mercury with the exception of those specified elsewhere in this Annex		
Classification according to Annex IV of the Regulation (EC) 790/2009	Classification and labelling according to CLP Regulation, 1st ATP from Annex I of the Regulation (EC) 790/2009	
	Hazard Class and Category Code(s)	Hazard statement Code(s)
T+; R26/27/28 R33 N; R50-53 Specific concentration limits: T+; R26/27/28: C ≥ 2 % T; R23/24/25: 0,5 % ≤ C < 2 % Xn; R20/21/22: 0,05 % ≤ C < 0,5 % R33: C ≥ 0,05 % (EC, 2008)	Acute Tox. 2 *: Acute toxicity (inhal.), hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) Acute Tox. 1: Acute toxicity (dermal), hazard category 1 Acute Tox. 2 *: Acute toxicity (oral), hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) STOT RE 2 *: Specific target organ toxicity-repeated exposure, hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) Aquatic Acute 1; Hazardous to the aquatic environment, acute hazard category 1 Aquatic Chronic 1: Hazardous to the aquatic environment, chronic hazard category 1 Specific concentration limit: STOT RE 2: H373 C ≥ 0.1%	H330: Fatal if inhaled H310: Fatal in contact with skin H300: Fatal if swallowed H373**: May cause damage to organs (or state all organs affected, if known) through prolonged or repeated exposure (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard). (** meaning Route of exposure cannot be excluded, see Annex VI, chapter 1.2.2 of the CLP Regulation) H400: Very toxic to aquatic life H410: Very toxic to aquatic life with long lasting effects.

Phenylmercury 2-ethylhexanoate CAS No. 13302-00-6 EINECS No. 236-326-7 EINECS Name: (2-ethylhexanoato)phenylmercury Included in index 080-004-00-7 “organic compounds of mercury with the exception of those specified elsewhere in this Annex		
Classification according to Annex IV of the Regulation (EC) 790/2009	Classification and labelling according to CLP Regulation, 1st ATP from Annex I of the Regulation (EC) 790/2009	
	Hazard Class and Category Code(s)	Hazard statement Code(s)
T+; R26/27/28 R33 N; R50-53 Specific concentration limits: T+; R26/27/28: C ≥ 2 % T; R23/24/25: 0,5 % ≤ C < 2 % Xn; R20/21/22: 0,05 % ≤ C < 0,5 % R33: C ≥ 0,05 % (EC, 2008)	Acute Tox. 2 *: Acute toxicity (inhal), hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) Acute Tox. 1: Acute toxicity (dermal), hazard category 1 Acute Tox. 2 *: Acute toxicity (oral.), hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) STOT RE 2 *: Specific target organ toxicity-repeated exposure, hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) Aquatic Acute 1; Hazardous to the aquatic environment, acute hazard category 1 Aquatic Chronic 1: Hazardous to the aquatic environment, chronic hazard category 1 Specific concentration limit: STOT RE 2: H373 C ≥ 0.1%	H330: Fatal if inhaled H310: Fatal in contact with skin H300: Fatal if swallowed H373**: May cause damage to organs (or state all organs affected, if known) through prolonged or repeated exposure (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard). (** meaning Route of exposure cannot be excluded, see Annex VI, chapter 1.2.2 of the CLP Regulation) H400: Very toxic to aquatic life H410: Very toxic to aquatic life with long lasting effects.

Phenylmercuric octanoate CAS No. 13864-38-5 EINECS No. No data found EINECS name. No data found Included in index 080-004-00-7 “organic compounds of mercury with the exception of those specified elsewhere in this Annex		
Classification according to Annex IV of the Regulation (EC) 790/2009	Classification and labelling according to CLP Regulation, 1st ATP from Annex I of the Regulation (EC) 790/2009	
	Hazard Class and Category Code(s)	Hazard statement Code(s)
T+; R26/27/28 R33 N; R50-53 Specific concentration limits: T+; R26/27/28: C ≥ 2 % T; R23/24/25: 0,5 % ≤ C < 2 % Xn; R20/21/22: 0,05 % ≤ C < 0,5 % R33: C ≥ 0,05 % (EC, 2008)	Acute Tox. 2 *: Acute toxicity (inhal.), hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) Acute Tox. 1: Acute toxicity (dermal), hazard category 1 Acute Tox. 2 *: Acute toxicity (oral.), hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) STOT RE 2 *: Specific target organ toxicity-repeated exposure, hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) Aquatic Acute 1; Hazardous to the aquatic environment, acute hazard category 1 Aquatic Chronic 1: Hazardous to the aquatic environment, chronic hazard category 1 Specific concentration limit: STOT RE 2: H373 C ≥ 0.1%	H330: Fatal if inhaled H310: Fatal in contact with skin H300: Fatal if swallowed H373**: May cause damage to organs (or state all organs affected, if known) through prolonged or repeated exposure (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard). (** meaning Route of exposure cannot be excluded, see Annex VI, chapter 1.2.2 of the CLP Regulation) H400: Very toxic to aquatic life H410: Very toxic to aquatic life with long lasting effects.

Phenylmercury neodecanoate CAS No. 26545-49-3 EINECS No. 247-783-7 EINECS Name neodecanoato-O)phenylmercury Included in index 080-004-00-7 “organic compounds of mercury with the exception of those specified elsewhere in this Annex		
Classification according to Annex IV of the Regulation (EC) 790/2009	Classification and labelling according to CLP Regulation, 1st ATP from Annex I of the Regulation (EC) 790/2009	
	Hazard Class and Category Code(s)	Hazard statement Code(s)
T+; R26/27/28 R33 N; R50-53 Specific concentration limits: T+; R26/27/28: C ≥ 2 % T; R23/24/25: 0,5 % ≤ C < 2 % Xn; R20/21/22: 0,05 % ≤ C < 0,5 % R33: C ≥ 0,05 % (EC, 2008)	Acute Tox. 2 *: Acute toxicity (inhal.), hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) Acute Tox. 1: Acute toxicity (dermal), hazard category 1 Acute Tox. 2 *: Acute toxicity (oral), hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) STOT RE 2 *: Specific target organ toxicity-repeated exposure, hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) Aquatic Acute 1; Hazardous to the aquatic environment, acute hazard category 1 Aquatic Chronic 1: Hazardous to the aquatic environment, chronic hazard category 1 Specific concentration limit: STOT RE 2: H373 C ≥ 0.1%	H330: Fatal if inhaled H310: Fatal in contact with skin H300: Fatal if swallowed H373**: May cause damage to organs (or state all organs affected, if known) through prolonged or repeated exposure (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard). (** meaning Route of exposure cannot be excluded, see Annex VI, chapter 1.2.2 of the CLP Regulation) H400: Very toxic to aquatic life H410: Very toxic to aquatic life with long lasting effects.

Methylmercury CAS No. 22967-92-6 EINECS No. Not available EINECS name: Methylmercury		
Methylmercuric chloride CAS No. 115-09-3 EINECS No. 204-064-2 EINECS name: Methylmercury chloride		
The classification of methylmercury and methylmercuric chloride was concluded in the former TC C&L group in exECB. They are included with index number 999-325-00-0. The classification and labelling according to Directive 67/548/EEC was concluded. Classification according to CLP are performed using the translation table from classification under directive 67/548/EEC, CLP Annex VII.		
Classification according to Annex IV of the Regulation (EC) 790/2009	Classification and labelling according to CLP Regulation, 1st ATP from Annex I of the Regulation (EC) 790/2009	
	Hazard Class and Category Code(s)	Hazard statement Code(s)
T+; R26/27/28 T; R48/25 Muta Cat 3; R68 Carc Cat 3; R40 Repr Cat 1; R61 Repr Cat 3; R62 R64 N; R50/53	Acute Tox. 2 *: Acute toxicity (inhal.), hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) Acute Tox. 1: Acute toxicity (dermal), hazard category 1 Acute Tox. 2 *: Acute toxicity (oral), hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) STOT RE 1: Specific target organ toxicity – repeated exposure, hazard category 1 Muta. 2: Germ cell mutagenicity, Hazard category 2 Carc. 2: Carcinogenicity, Hazard Category 2 Repr. 1B:Reproductive toxicity, Hazard category 1B Repr. 2: Reproductive toxicity, Hazard category 2. Lact: Reproductive toxicity, Additional category, Effects on or via lactation	H330: Fatal if inhaled H310: Fatal in contact with skin H300: Fatal if swallowed H372**: Causes damage to organs (state all organs affected, if known) through prolonged or repeated exposure (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard) (** meaning Route of exposure cannot be excluded, see Annex VI, chapter 1.2.2 of the CLP Regulation) H341: Suspected of causing genetic defects (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard) H351: Suspected of causing cancer (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard) H360D: May damage the unborn child

	Aquatic Acute 1: Hazardous to the aquatic environment, acute hazard category 1 Aquatic Chronic 1: Hazardous to the aquatic environment, chronic hazard category 1	H361f: Suspected of damaging fertility H362: May cause harm to breast-fed children H400: Very toxic to aquatic life H410: Very toxic to aquatic life with long lasting effects

Mercury dichloride CAS No. 7487-94-7 EINECS No. 231-299-8 EINECS name: Mercury dichloride Included with index number 080-010-00-X for mercury dichloride.		
Classification according to Annex IV of the Regulation (EC) 790/2009	Classification and labelling according to CLP Regulation, 1st ATP from Annex I of the Regulation (EC) 790/2009	
	Hazard Class and Category Code(s)	Hazard statement Code(s)
T+; R28 T; R48/24/25 C; R34 Muta Cat 3; R68 Repr Cat 3; R62 N; R50/53	Acute tox 2*: Acute toxicity (oral), Hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) Skin Corr. 1B: Skin corrosion/irritation, hazard category 1B. STOT RE 1: Specific target organ toxicity- repeated exposure, hazard category 1 Muta 2: Germ cell mutagenicity, Hazard category 2. Repr. 2: Reproductive toxicity, Hazard category 2. Aquatic Acute 1: Hazardous to the aquatic environment, acute hazard category 1 Aquatic Chronic 1: Hazardous to the aquatic environment, chronic hazard category 1	H300: Fatal if swallowed H314: Causes severe skin burns and eye damage H372**: Causes damage to organs (state all organs affected, if known) through prolonged or repeated exposure (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard). (** meaning Route of exposure cannot be excluded, see Annex VI, chapter 1.2.2 of the CLP Regulation) H341: Suspected of causing genetic effects (state route of exposure if it is conclusively proven that no other routes of exposure cau se the hazard) H361f***: Suspected of damaging fertility (***meaning the general hazard statement can be replaced by the hazard statement indicating only the property of concern, where either fertility or developmental effects are proven to be not relevant, see Annex VI, chapter 1.2.3 of the CLP Regulation) H400: Very toxic to aquatic life H410: Very toxic to aquatic life with long lasting effects

Mercury CAS No: 7439-97-6 EC No: 231-106-7 Index No: 080-001-00-0		
Classification according to Annex IV of the Regulation (EC) 790/2009	Classification and labelling according to CLP Regulation, 1st ATP from Annex I of the Regulation (EC) 790/2009	
	Hazard Class and Category Code(s)	Hazard statement Code(s)
T+; R26 T; R48/23 Repr. Cat. 2; R61 N; R50-53 Note E: The R phrases indicating specific effects on human health shall be preceded by the word 'Also'.	Acute Tox. 2*: Acute toxicity (inhal.), hazard category 2 (* meaning Minimum classification, see Annex VI, chapter 1.2.1 of the CLP Regulation) STOT RE 1: Specific target organ toxicity – repeated exposure, hazard category 1 Repr. 1B: Reproductive toxicity, hazard category 1B Aquatic Acute 1: Hazardous to the aquatic environment, acute hazard category 1 Aquatic Chronic 1: Hazardous to the aquatic environment, chronic hazard category 1	H330: Fatal if inhaled H372**: Causes damage to organs (state all organs affected, if known) through prolonged or repeated exposure (state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard) (** meaning Route of exposure cannot be excluded, see Annex VI, chapter 1.2.2 of the CLP Regulation) H360D***: May damage fertility or the unborn child (***meaning the general hazard statement can be replaced by the hazard statement indicating only the property of concern, where either fertility or developmental effects are proven to be not relevant, see Annex VI, chapter 1.2.3 of the CLP Regulation) H400: Very toxic to aquatic life H410: Very toxic to aquatic life with long lasting effects

Appendix 8. Mercury monitoring data

This section presents monitoring data on mercury in general.

Measured environmental concentrations and trends
Mercury is known to circulate between the earth's different environmental compartments through a complex biogeochemical cycle, and human activity has introduced additional processes that have increased the rate of distribution between the compartments (Stein et al., 1996). Environmental cycling of mercury can be described as a series of processes where chemical, biological and physical transformations are governing the factors controlling the distribution of mercury in and between different environmental compartments. Briefly, the global cycling involves natural and anthropogenic emission, dispersion in the atmosphere where chemical transformation may occur, dry and wet deposition to aquatic and terrestrial surfaces and finally re-emission (Baeyens, 1992, Mason et al., 1994). In the Arctic, mercury has an especially complex cycle including a unique scavenging process (mercury depletion events), biomagnifying food webs, and chemical transformations such as methylation.

Mercury (Hg) is emitted to the atmosphere by a variety of natural (volcanoes, wildfires, etc.) and anthropogenic (e.g., combustion of coal) sources (Nriagu and Pacyna, 1988). While anthropogenic Hg emissions have decreased over North America and Europe during the 1990s, emissions in Asia have strongly increased and China is now the country with the by far largest Hg emissions worldwide (Pacyna et al., 2006). Once released into the atmosphere, mercury can undergo long-range atmospheric transport hence the atmosphere is the most important pathway for the worldwide dispersion and transport of mercury in the environment (Cheng and Schroeder, 2000). In the atmosphere, Hg exists predominantly as gaseous elemental mercury (GEM), which under normal conditions is relatively inert, allowing for homogenous mixing within each hemisphere. GEM can be converted to various oxidized compounds in the gas or particulate phase, which have a much shorter atmospheric lifetime than GEM.

The Arctic is believed to be a global sink of mercury due to a set of extraordinary circumstances occurring during Polar spring where GEM is rapidly oxidized following sudden depletion in the atmosphere (Figure B9.2). This phenomenon, termed atmospheric mercury depletion events (AMDE), is a circum polar phenomenon. During AMDEs, GEM is transformed into oxidized forms through a chain of photochemical and heterogeneous processes. These oxidized forms are quickly lost from the atmosphere resulting in large seasonal fluxes of Hg onto snow and ice surfaces (e.g., Lindberg et al., 2002; Steffen et al., 2008).

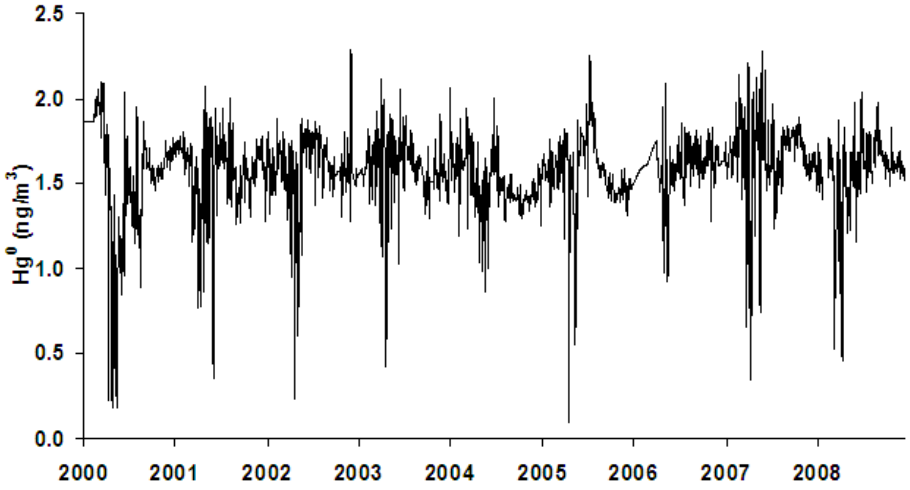


Figure B9.2: Time series of gaseous elemental mercury from Ny-Ålesund (Svalbard) showing the reoccurring Polar spring phenomena atmospheric mercury depletion events (source NILU).

Spatial and temporal trends for long range transported mercury

Several long-term mercury monitoring networks have been established, monitoring the concentration of Hg in wet deposition and air. E.g., in Europe monitoring of mercury air concentrations and deposition are carried out within the framework of the Cooperative Program for Monitoring and Evaluation of the Long-range Transmission of Air Pollutants in Europe (EMEP), whereas the Arctic Monitoring and Assessment Programme (AMAP) is responsible for a coordinated air monitoring program that covers the circum-Arctic areas of North America and Eurasia. However, even the longest established monitoring programs can only provide data on air concentration and deposition of mercury for the last 15 to 20 years. Natural environmental archives such as lake sediments, peat and ice cores are therefore the only link between current and past loading to terrestrial and aquatic environments. These archives provide a useful means of reconstructing the atmospheric load on a local, regional and global scale (Biester et al., 2007). In both peat and lake sediment cores, a clear increase in mercury concentration are observed today compared to pre-industrial times. E.g., in sediments the peak concentrations are found in samples dating to the 1970s to 1990s, in agreement with emission inventories. Ice cores have produced a similar result, with 70% of deposited mercury found to be of anthropogenic origin (Schuster et al., 2002).

Air: Global trend data

Long-term monitoring data series for Hg in air are sparse therefore data have been pooled to estimate global trends. The background concentration of GEM in the northern hemisphere is between 1.5 and 1.7 ng/m3, and between 1.1 and 1.3 ng/m3 in the southern hemisphere (Slemr et al., 2003). A decreasing concentration trend has been observed at some monitoring stations, e.g. Rørvik (Sweden) (Wangberg et al., 2007) and stations close to population centers in Toronto and Montreal (Canada) (Temme et al., 2007). Although such regional decreases in concentration of mercury in air have been observed, the global background concentration of GEM in air has remained constant over the past 20 year. Analysis of GEM concentration values reveal a relatively stable level over the period 1977 to 2002 (AMAP/UNEP 2008). Analysis of the longest Arctic GEM time series (from Alert, Canada

and Ny-Ålesund, Norway) shows no significant change in concentration level (Temme et al., 2007, Berg et al., 2009).

Precipitation
Anthropogenic emissions of mercury have changed dramatically during the last 70 years (Pacyna et al., 1995, 2006). Emissions of mercury to the atmosphere, in particular from industrial point sources, have decreased significantly in Europe and North America, whereas they have increased in East Asia. It is therefore important to see how concentrations and wet and dry deposition have responded to these changes. Measurements of mercury in precipitation go back to the 1980s, and both precipitation amount and concentrations of mercury in precipitation have been measured worldwide. Concentrations on Europe and North America have generally decreased (AMAP/UNEP, 2008). Such a decrease is observed e.g at Rørvik, Sweden, where concentrations in rain water have decreased from 50 ng/l in the 1980s to 15 ng/l in the 2000s, which coincide with decreases in European emissions (Wängberg et al., 2007). Trend analysis of Hg deposition from Lista (and Birkenes) in Norway shows a significant decrease in Hg deposition during 19 years of measurements. The decrease is about 0.5 µg Hg/m2 * year (Aas et al., 2008).

Lake sediments
Lake sediment cores from remote areas in temperate and boreal areas and the Arctic are studied as archives for Hg deposition (Ranneklev et al, 2009). In general, the cores reveal an increase in Hg from past to present, with a particular increase after the onset of the Industrial Revolution, with a peak in the late 20th century. The last 10-15 years, Hg contents in lake sediments have gradually declined, probably due to reduced emissions. The ratio of Hg between surfaces to deep cores not influenced by industrial deposits is referred to as the enrichment factor (EF), where EF > 1 indicates influence by external sources. Enrichment factors of 1.1 to 30 are reported, but the most common values are roughly between 1.3 and 6. Generally, sediment enrichment of Hg is highest in regions with highest atmospheric deposition.

A study of 110 lakes at mainland Norway and Svalbard (Arctic) showed that Hg in lake sediments is on average elevated compared to pre-industrial times, with lakes in the south being more elevated compared to lakes in the northern part of Norway and Svalbard. The highest levels of Hg in the Svalbard lakes were recorded in lakes that are influenced by seabirds. The concentrations in the lakes in the circum-Arctic areas of North America and Eurasia are low compared to levels in the southern part of Norway (Rognerud et al. 2008). Changes in lake sediment concentrations in recent time reveal a slight increase in concentrations. The increase is associated to atmospheric long-range transport. The largest increase occurs along the coast, in southern Norway and in eastern Finnmark. There are apparently no changes in the Svalbard lakes.

Mosses and lichens
Mosses and lichens are excellent biomonitors of atmospheric deposition due to their lack of root system (Steinnes, 1995). Sampling and analysis of mosses and lichens are an established method for studying atmospheric deposition on large geographical scales, and in Norway, such monitoring of heavy metal deposition have been undertaken every 5th year since 1975. The level and geographical distribution of mercury in mosses were relatively constant from 1985-1995, whereas a general decrease was observed in 2000. Results from 2005 are similar to the results from 2000 (Steinnes et al, 2007).

Spatial and temporal trend for mercury in biota

In the environment, particularly lakes, waterways and wetlands, mercury can be converted to MeHg through biogeochemical interactions. As MeHg, mercury bioaccumulate and biomagnify through the food chain, and levels of mercury in different organism depend on trophic level, size and age of the organism. Levels also vary by species and location. Bioaccumulation in fish is influenced by the amount of methylmercury present, which is in turn affected by local biogeochemical processes and by mercury inputs from atmospheric pollution. According to EU-regulations the Hg-content in fish commercially available should not exceed 0.5 mg/kg. In order to limit human exposure to mercury from contaminated fish, authorities worldwide have issued fish consumption advisories for a large number of water bodies. Most of the mercury found in biota is present as MeHg. In some cases, methylmercury levels in carnivorous fish, such as freshwater bass, walleye and pike, and marine shark and swordfish, bioaccumulate up to a million times greater than in the surrounding water. Although fish appear to be tolerant to large body burdens of methylmercury, there have been human deaths in cases of severe poisoning, e.g. the severe Minamata bay disaster (e.g. Ishimure, 2003) and Iraq mercury poisoning (e.g. Engler, 1985).

Mercury levels in fish

Concentrations of mercury in fish in Scandinavia and North America are frequently above the limit recommended for human consumption. ICP Waters Programme Centre has recently summarized this information (Ranneklev et al, 2009): Levels of Hg in fish vary with species, size, age, differences in Hg exposure, food web structure, and dietary strategy. Surveys of Hg in fish from various regions follow different designs, and collecting of supporting data that allow interpretation of results in relation to key controlling factors is done to varying degrees. Thus, differences in Hg levels in fish sampled in different surveys may be controlled by fish size or position in the aquatic food web rather than by differences in Hg deposition. However, highest concentration of mercury in fish is often found in iscivorous fish species and top predators. In Scandinavia and North America elevated concentrations of Hg is often found in Northern pike and perch, and the concentrations are often above the limit recommended for human consumption. Compiled results on Hg from Scandinavia have shown that Northern pike caught in Scandinavia has slightly elevated levels of Hg compared to North America. For perch, the concentrations are comparable or somewhat lower in Scandinavia. Mercury concentrations in surface waters in remote areas are usually lower than the WFD environmental quality standard (EQS) (0.05 μg/l). However, many of these waters have fish with Hg concentrations substantially higher than recommended limits for human consumption (a maximum level of 0.5 mg/kg mercury applies to fishery products, with the exception of certain listed fish species for which 1 mg/kg applies) and the WFD EQS for Hg in fish (0.02 mg/kg). Thus, the concern with regard to Hg pollution and human and wildlife exposure to Hg is not addressed satisfactorily with the EQS for Hg in water under WFD. The EQS for Hg in fish (0.020 mg/kg wet weight), on the other hand, is exceeded for most fish all over Scandinavia.

Data on mercury levels in freshwater fish from Sweden have been collected from more than 2000 lakes (Åkerblom and Johansson, 2008). The data show a significant regional gradient with higher levels in the southern part compared to the northern part. In the southern parts the levels are generally between 0.5 and 1.0 mg/kg wet weight whereas the levels in the northern part generally are lower than 0.25 mg/kg. This gradient follows in general the pattern of atmospheric depositions.

A downward trend was apparent in the 1980´ies and the levels where more or less stable during the 1990´íes. However, during the last decade there has been an increasing trend in the mercury levels in inland fish in the majority of lakes in Sweden. Although the atmospheric depositions has declined, the depositions are still high and they contribute to a slowly increasing level in soil. This in turn implies an increasing run-off and load on aquatic systems. Climate changes might also be a contributing factor. The levels in fish are currently about 3-5 higher than the estimated background levels (Åkerblom and Johansson, 2008).

In a study of Hg in fish from Norwegian lakes it was concluded that there are large regional differences in the Hg-concentration, with generally higher Hg-concentrations in the southern part compared to the north, with the lowest concentrations in the Arctic(Christensen et al., 2008). Norwegian authorities have issued fish consumption advisories for especially fish from Mjøsa, the largest lake in Norway, due to the high mercury content. Based on data from 2006–2008, the average mercury content in brown trout larger than 55 cm or 1.9 kg from lake Mjøsa will exceed the consumption limits of 0.5 mg/kg (Fjeld et al., 2009).

For lake Mjøsa in particular, the length adjusted mean mercury concentrations (mean length ≈ 56 cm, mean weight ≈ 2 kg) in brown trout was reduced from 1.39 mg/kg in a survey from 1979–1980 to 0.36 mg/kg in survey carried out in 1982–1984. A decreasing trend was found up to 2005 (0.36 mg/kg), but then the concentrations in 2006–2008 increased again to a higher level of about 0.53 mg/kg (Fjeld et al., 2009).

In a study of trout from 17 different Norwegian lakes the concentration of mercury was determined in 223 trout, of which the populations in 14 of these had been investigated for mercury in the period 1988–2001.For the 14 stocks in which a comparison with previous data was possible, samples consisted of 177 fish caught in 2008 and 264 fish caught during the period 1988-2001. The concentrations in 2008 were statistically significantly higher for eight of the 14 populations, while a significant reduction could be detected for one population. On average, the concentration had increased by approximately 23%, from 0.118 mg / kg to 0.145 mg / kg. According to the EU's Water Framework Directive, the environmental quality requirements for fish and other aquatic biota are set to 0.02 mg Hg/kg (wet weight) or less. All of the analyzed fish samples from 2008 exceeded this limit. (Fjeld and Rognerud, 2009a).

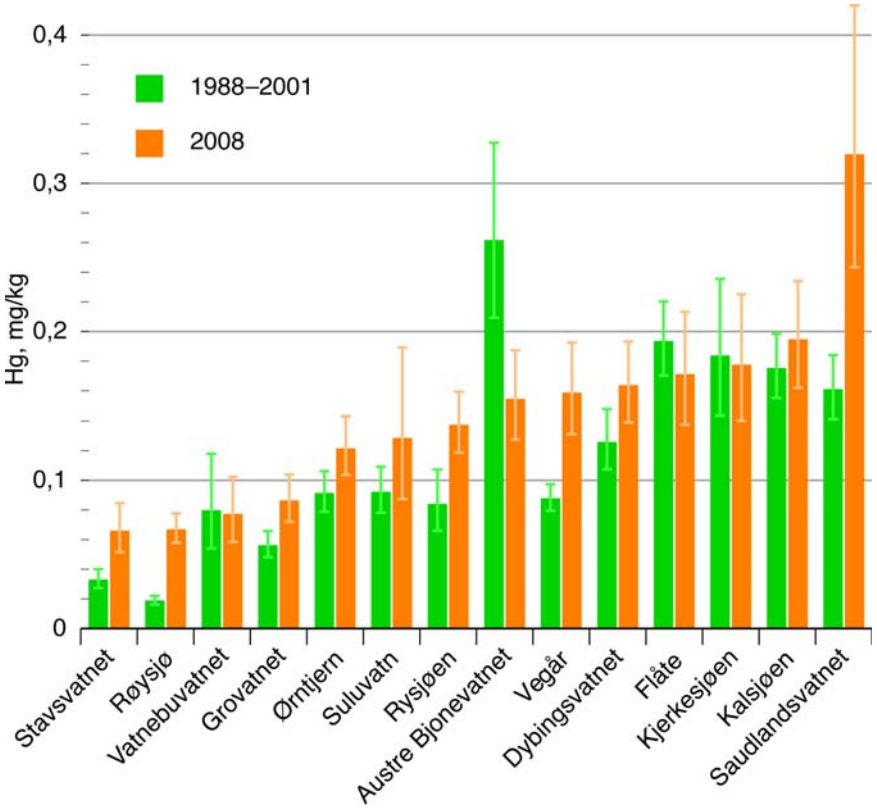


Figure B9.3. Mean adjusted mercury concentrations in trout caught in 2008 and in the period 1988–2001. The concentrations are adjusted for length and are calculated relative to fish where the length is the geometric mean for the whole sample. Vertical bars indicate 95 % confidence intervals.

In another study the mercury concentrations were determined in 565 perch (Perca fluviatilis) from 28 lakes in South-East Norway (Fjeld and Rognerud, 2009b). The concentrations increased with fish size, and in average the EU's consumption limit of 0.5 mg Hg/kg (wet weight) were exceeded at a fish size of approximately 24 cm, or 200 g. The highest concentrations were primarily found in populations from forest lakes in the eastern part of the region. The length adjusted average mercury concentration in ten perch populations increased with 63% from 1991 to 2008. In eight of the ten re-sampled lakes a statistically significant increase in the fish mercury concentrations was proved ($p < 0.05$).

According to the authors this increase is unexpected as no local mercury sources exist in the precipitation area of the lakes and the atmospheric mercury depositions have decreased in South-East Norway since the beginning of the 1990s. Mercury in fish exists mainly as methylmercury, and factors stimulating the mercury methylation, such as a warmer and wetter climate and also forestry and lumbering, may have contributed to the observed increase.The influence of these factors are now further investigated.

Fish eating predators

Mercury has always been present in the Arctic but levels in many areas of the Arctic are considerably higher now than they were before the beginning of the industrial era. Fish eating predators such as osprey, eagles, northern pike and kingfishers, generally have high concentrations of mercury. Mercury has been detected in Common Loons from Alaska to Atlantic Canada, and blood concentrations have been correlated with levels in prey fish species. A general spatial distribution pattern of mercury content in terrestrial animals show

that concentrations are usually higher in Alaska, Canada and West Greenland whereas lower in Scandinavia and Russia (AMAP, 2004). E.g., concentrations of mercury in ptarmigan liver showed in Scandinavia high variability and no distinct regional pattern, while in Canada higher concentrations were observed in central and western regions (Figure B9.4). Similarly, the highest mercury concentrations in reindeer/caribou liver were found in northern Quebec, south-west Greenland and Alaska, whereas in Scandinavia and Russia concentrations were mostly lower. As for marine invertebrates, e.g., blue mussel, no circum polar trend was apparent. A study of seabirds within the Norwegian Arctic showed that concentrations of mercury in the liver of glaucous gull and great-black backed gulls were comparable to levels reported in other Arctic seabird species (Knudsen et al., 2007). However, in northern fulmar, the levels of mercury were high compared to other Arctic seabird species. The levels were below reported lethal threshold levels in birds, but close to levels associated with malnutrition and chronic diseases in other seabird species (Gabrielsen et al., 2005).

Levels of mercury in eggs from four seabird species (herring gulls, Atlantic puffins and black-legged kittiwakes from Northern Norway and glaucous gulls from Bjørnøya (Svalbard)) showed no significant spatial variation or temporal trend in eggs collected in the period 1983-2003 (Knudsen et al., 2005.). In a study of ivory gull eggs from four different bird colonies in the Norwegian and Russian Arctic there was no difference in the level of mercury between colonies (Miljeteig et al., 2007).

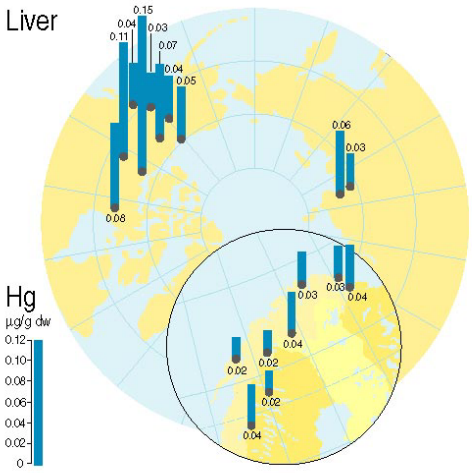


Figure B9.4: Circumpolar levels of Hg in liver tissue of ptarmigan (Source AMAP 1998. AMAP Assessment Report: Arctic Pollution Issues. Arctic Monitoring and Assessment Programme (AMAP), Oslo, Norway. Xii+859 pp).

Marine mammals

The importance of monitoring contaminant concentrations in marine mammals cannot be overstated, as they are key dietary routes for human exposure to Hg in many Arctic communities. However, they are not ideal environmental monitors of ambient conditions as they are long-lived, and therefore bioaccumulate and depurate contaminants throughout their lives. The age-adjusted total mercury content in ringed seal liver indicates a different spatial trend to the generally declining west-to-east pattern across Arctic North America. Hg levels in ringed seal liver were lower in Alaska compared to the eastern Canadian Arctic, whereas seals collected in northern and western Greenland appeared lower than in the eastern Canadian Arctic. Ringed seal from Svalbard had the lowest Hg content (AMAP, 2004).

Temporal trend for mercury in the ArcticWhere available, temporal trend data for biota in terrestrial, freshwater and marine environments show trends that are not always consistent with those observed in abiotic compartments, such as ice and sediments. Data from the past few decades show that mercury levels are increasing in some Arctic biota, in particular in marine birds and mammals from areas in Canada and West Greenland (AMAP 2007). The annual average increase is between 1.9 to 10%. By contrast, mercury levels in the marine environment around Iceland and in the sub-arctic terrestrial and freshwater environments of Scandinavia, a general decrease in mercury levels in biota is observed. In particular, there seem to be no significant changes in mercury levels in marine species from the Barents Sea area since the 1990s (Jæger et al., 2007). Long-term data sets for human teeth and hair show that total Hg concentrations increased between the pre-industrial era and modern times (1970s) although there is evidence to suggest that Hg concentrations in Norwegians have decreased substantially since then (AMAP, 2004). Recent research show that mercury in predators occupying top levels of the Arctic food chain is almost exclusively methylated (Campbell et al., 2005) and that blood and fatty tissue of native human populations have elevated levels of mercury (Bjerregaard and Hansen, 2000, Van Oostdam et al., 2005) which clearly indicate that the dynamics and impact of mercury contamination in the Arctic are similar to these phenomena in temperate zones of the world. Current mercury exposure poses a significant health risk for Arctic indigenous people, especially the Inuit population at Greenland and Northwest Canada, who mainly feed on local food sources such as seal, whale and fatty fish. These people have a daily methylmercury intake higher than recommended by WHO (AMAP, 2002). In these areas, more children than normal are borne with learning disabilities as a result of their mothers' high mercury blood content.

Appendix 9. Pre-registered phenylmercury compounds

List of pre-registered substances
Your query returned 33 matching records.
All substances without an existing EC number have been given a listnumber in the EC format.
Listnumbers have been provided to make registration easier.
Substances without an EC number, but with a CAS number appear in the list in green, preceded by a *.
Substances without an EC number or a CAS number (these were identified by name or as multiconstituent substances) appear in red, preceded by a @.

EC Number	CAS Number	Name	Synonym	Envisaged registration deadline	Related substances
200-242-9	55-68-5	phenylmercury nitrate		30/11/2010	-
200-532-5	62-38-4	phenylmercury acetate		30/11/2010	-
202-331-8	94-43-9	phenylmercury benzoate		30/11/2010	-
202-865-1	100-56-1	phenylmercury chloride		30/11/2010	-
202-866-7	100-57-2	phenylmercury hydroxide		30/11/2010	-
203-068-1	102-98-7	dihydrogen [orthoborato(3-)-O]phenylmercurate(2-)		30/11/2010	-
203-094-3	103-27-5	phenylmercury propionate		30/11/2010	-
203-217-0	104-59-6	phenylmercury stearate		30/11/2010	-
203-218-6	104-60-9	(oleato)phenylmercury		30/11/2010	-

204-560-9	122-64-5	lactatophenylmercury		30/11/2010	-
209-534-0	584-18-9	2-hydroxy-5-(1,1,3,3-tetramethylbutyl)phenylmercury acetate		30/11/2010	-
209-606-1	587-85-9	diphenylmercury		30/11/2010	-
214-760-8	1192-89-8	bromophenylmercury		30/11/2010	-
218-909-8	2279-64-3	(phenylmercurio)urea		31/05/2013	-
220-286-2	2701-61-3	(maleoyldioxy)bis[phenylmercury]		31/05/2013	-
221-961-4	3294-58-4	(bromodichloromethyl)phenylmercury		30/11/2010	-
228-497-1	6283-24-5	4-aminophenylmercury acetate		30/11/2010	-
236-326-7	13302-00-6	(2-ethylhexanoato)phenylmercury		31/05/2013	-
245-006-6	22450-90-4	amminephenylmercury(1+) acetate		30/11/2010	-
245-581-3	23319-66-6	[2,2',2"-nitrilotri(ethanol)-N,O,O',O"]phenylmercury lactate		31/05/2013	-
247-783-7	26545-49-3	(neodecanoato-O)phenylmercury		30/11/2010	4
248-426-8	27360-58-3	(dihydroxyphenyl)phenylmercury		31/05/2013	-

248-559-1	27605-30-7	[2-ethylhexyl hydrogen maleato-O']phenylmercury		31/05/2013	-
248-828-3	28086-13-7	phenylmercury salicylate		31/05/2013	-
250-518-8	31224-71-2	(metaborato-O)phenylmercury		31/05/2013	-
250-736-3	31632-68-5	[naphthoato(1-)-O]phenylmercury		31/05/2013	-
251-026-6	32407-99-1	phenylmercury dimethyldithiocarbamate		31/05/2013	-
263-211-9	61792-06-1	[(2-hydroxyethyl)amino]phenylmercury acetate		31/05/2013	-
269-247-1	68201-97-8	(acetato-O)diamminephenylmercury		30/11/2010	-
301-792-3	94070-93-6	[μ-[(oxydiethylene phthalato)(2-)]]diphenylmercury		30/11/2010	-
@906-798-5		Reaction mass of (neodecanoato-O)phenylmercury and butane-1,4-diol		31/05/2018	-
@911-619-9		Reaction mass of (neodecanoato-O)phenylmercury and 3-isocyanatomethyl-3,5,5-trimethylcyclohexyl isocyanate		31/05/2018	-
@915-515-4		Reaction mass of (neodecanoato-O)phenylmercury and neodecanoic acid		31/05/2018	-

Related substances for (neodecanoato-O)phenylmercury
EC Number: 247-783-7, CAS Number: 26545-49-3
Please note, that to use all features on this page, you must enable JavaScript in your browser!
Related substances are substances which might be used for (Q)SAR, grouping (or category approach) and read-across (REACH regulation, Annex XI; Section 1.3 and 1.5). Please note that they are solely based on proposals made by pre-registrants.

EC Number	CAS Number	Name
200-242-9	55-68-5	phenylmercury nitrate
200-532-5	62-38-4	phenylmercury acetate
202-866-7	100-57-2	phenylmercury hydroxide
236-326-7	13302-00-6	(2-ethylhexanoato)phenylmercury

Appendix 10. Analytical methods (mercury)

Analytical methods for testing plastic materials

Monitoring of the 5 proposed phenylmercury compounds in articles is suggested by measurement of mercury concentration (% of Hg) in the articles, or parts of articles. This has several reasons:

Until now, no reliable, sensitive and selective procedures have been developed to measure concentrations of the 5 phenylmercury carboxylates in articles. One method on the measurement of phenylmercury acetate in coatings is published, however, this method is not validated in ring tests and sufficiently quality assured. Thus, if considered necessary, methods have to be further developed and validated for the 5 proposed phenylmercury carboxylates.

It cannot be ruled out that phenylmercury carboxylates are partly degraded in articles either during processing or due to photolytic degradation in finished articles. The published literature does not provide evidence to which extent phenylmercury compounds are degraded in the articles to elemental mercury prior to volatilizing, or if it is converted to elemental mercury in air. This question needs additional research (ATSDR, 2008). Principally, degradation can also occur in the articles.

Portable field instruments provide easy, reliable and sensitive measurement of mercury in articles, and thus are well-suited tools for screening articles. Several laboratory methods are available for quantification of mercury in plastics (see below). Determination of mercury concentration (% of Hg) is in line with the EC Regulation on cosmetic products (Regulation EC/1223/2009) where some mercury compounds, including phenylmercury acetate, are allowed for use as preservative. The concentration limit is expressed in terms of mercury (0.007 % of Hg) and if mixed with other mercurial compounds authorized the maximum concentration of Hg remains fixed at 0.007% Hg.

Measurement of mercury in plastic samples

Several methods exist to measure mercury content in articles:

Screening method:

Screening of mercury in articles can be done using portable, easy-to-use X-ray fluorescence (XRF) analysers. The sensitivity varies between models, however, the limit of detection is well below 0.01 % for mercury in polymeric polyethylene (PE), polyvinyl chloride (PVC) and acrylonitrile butadiene styrene (ABS) thermoplastics. The limit of detection is 4-8 mg/kg in PE and 25-40 mg/kg in PVC

Laboratory methods

Hill and Santamaria-Fernandez (2009) (See: http://www.chem.agilent.com/Library/applications/5990-5059EN.pdf) presented a laboratory method for the quantification of cadmium, chromium, lead and mercury in plastic materials by external calibration using the Agilent 7500ce ICP-MS system equipped with an Octopole Reaction System (ORS). Microwave digestion was employed to ensure complete dissolution of the sample. Isotope dilution analysis with ICP-MS was used as a confirmatory technique. Good agreement of the results obtained by two different calibration approaches was achieved. The method validated with isotope dilution mass spectrometryresults has potential as a fast analytical tool for compliance testing laboratories. The limit of detection is calculated to 0.10 ng/g (10-8 %), the limit of quantification is 17.2 µg/g (0.0017%).

US-EPA has published two test methods for the measurement of mercury in solid or semisolid waste.

Method 7471B (PDF) uses aqua regia (concentrated HCl and HNO3) or concentrated H2SO4 and HNO3 is used to extract mercury from the sample at elevated temperatures between 95 and 120oC. Cold-vapor atomic absorption spectrometry is used to analyse mercury in the extract. The typical instrument detection limit (IDL) for this method is 0.0002 mg/L. Alternatively, Method 7473 (PDF) can be used. Controlled heating in an oxygenated decomposition furnace is used to liberate mercury from solid samples in the instrument. The sample is dried and then thermally and chemically decomposed within the decomposition furnace. The mercury is selectively trapped in an amalgamator and after removal of decomposition products the amalgamator is heated and released mercury determined at 253.7 nm in an atomic absorption spectrophotometer. The instrument detection limit (IDL) for this method is 0.01 ng of total mercury.
The procedures can be found on the following website:
http://www.epa.gov/osw/hazard/tsd/mercury/tests.htm

Determination of phenylmercury in coatings and environmental samples
If the mercury concentration (% of Hg) in articles exceeds the proposed limit of 0.01%, the presence of phenylmercury carboxylates might be confirmed by more advanced laboratory analysis. For most of the proposed phenylmercury compounds no analytical procedures are published yet. However, several of the below mentioned methods can be adapted to detect the five proposed phenylmercury carboxylates.
One analytical procedure is published (Niu et al., 2007) describing the analysis of phenylmercury acetate in coatings by high performance liquid chromatography (HPLC). Coatings were extracted with acetonitrile in an ultrasonic blender and chromatographic separation was performed on a C18 column with 10% ammonium acetate (2 mM) in acetonitrile as the mobile phase. The detection was done with a diode-array-detector at 195 nm. The detection limit of the method is 0.097 mg/L (or 0.00243% of the extracted sample). Recoveries range from 97.3% to 103.1%, with relative standard deviation of less than 4.5% (n=7). According to the authors of the study, the method established is selective, sensitive, exact and completely satisfies high sensitive analysis for PMA in coating.
For the remaining 4 phenylmercury carboxylates no analytical procedure could be found. Other studies describe the analysis of phenylmercury compounds in other matrices like pharmaceutical products, soil, water and biota. Because in aqueous media phenylmercury carboxylates are dissociated into phenylmercury and the corresponding carboxylate, the analysis of phenylmercury is usually described.
A gas chromatographic determination method for inorganic mercury and organomercury in biological material using packed-column GC/ECD has been developed by Cappon and Smith (1977). Methyl-, ethyl-, and phenylmercury were first extracted as chloride derivatives and subjected to thiosulfate clean-up, and finally isolated as bromide derivatives. The method provides a detection limit of 1 ng/g or lower with a mean deviation of 3.2%.
Separation and determination of diethylmercury, methylmercury chloride, ethylmercury chloride and phenylmercury chloride using capillary GC with AAS detection has been achieved (Jiang et al., 1989). A OV-17 WCOT column (12 m x 0.3 mm) was used to separate the mercury compounds and the effluent from the column was led through a stainless steel pyrolyser kept at 700 oC and detected by AAS. The absolute detection limit was about 0.1 ng mercury. Another method coupling GC and AAS developed by Emteborg et al. (1999) employed a wide bore capillary GC column, on-line pyrolyser at 800 oC (to generate mercury atoms) and AAS detector in a quartz cuvette. The use of the 184.9 nm line provided a more than five-fold increase in sensitivity, compared with the conventional 253.7 nm line, and an absolute detection limit of 0.5 pg of mercury.

Bache et al. (1971) first applied GC/MED to organomercury compound. Using packed columns (60/80 Chromosorb 101, 20% OV-17/QF-l(1: I)), five organomercury compounds (dimethylmercury, methylmercuric chloride, methylmercuric dicyanodiamide, phenylmercuric acetate and methylmercury dithizonate) were separated.
Reversed-phase HPLC with UV detection was optimized for the simultaneous separation and quantification of nine organic mercury compounds: methyl-, ethyl-, phenyl-, methoxymethyl-, ethoxymethyl-, benzoic and toluylmercury, mersalylic acid and nitromersol (Hempel et al., 1991). The nine compounds were successfully separated on ODS columns by gradient elution with a methanol-water mixture ranging from 30% to 50% (v/v). The detection limits were in the range 70-95 ng/l.
Several HPLC methods have been utilized for the determination of mercurial compounds in pharmaceutical preparations. In addition to the methods mentioned before, the following procedures have been reported.
Larroque and Vian (1993) reported RP-HPLC with C18 column for the determination of phenylmercuric nitrate in pharmaceutical products. The detection was carried out using UV detector at 258 nm. The mobile phase was water, acetonitrile, and EDTA.
Parkin (1987) determined a number of phenylmercury salts in pharmaceutical products performing high-performance liquid chromatography of a morpholinedithiocarbamate derivative. The method is specific and sensitive.
An LC method with online UV irradiation was developed by Falter and Schöler (1994) for AAS. Methyl-, ethyl- , phenyl and inorganic Hg were separated on reversed phase C18 columns. A UV-irradiation lamp was used for the online destruction of the organomercury compounds. Samples and NaBH4 solution were continuously fed to the reaction vessel where Hg was reduced, and the volatilized Hg was swept with nitrogen into the absorption cell of a CVAAS system.
Extraction of phenylmercury carboxylates from plastics is preferably conducted with a polar extractant. According to Bolgar et al. (2008), polymers should be shredded and milled before extraction to increase the contact surface of the polymer. When extracted with water-free, organic extractants such as acetonitrile, phenylmercury carboxylates do not dissociate and can be determined as the undissociated molecule. Simple extraction of polymer with an organic solvent in an ultrasonic blender or a horizontal shaker might be sufficient to extract phenylmercury carboxylates from the polymer, however, more advanced methods like Soxhlet extraction or accelerated solvent extraction are preferred if the extraction efficiency is too low with the simple methods.

References

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Analytical methods for testing plastic materials

Screening methods:

X-ray fluorescence (XRF) analyzer
Sensitivity varies between models, limit of detection below 0.01 % for mercury is not problematic in polymeric polyethylene (PE), polyvinyl chloride (PVC) and acrylonitrile butadiene styrene (ABS) thermoplastics.
Limit of detection (examples): 4-8 mg/kg in PE and 25-40 mg/kg in PVC

Extraction method used commercially with common extraction methods:

Agilent 7500ce ICP-MS system equipped with an Octopole Reaction System (ORS) and Integrated Sample Introduction System (ISIS) (microwave digested samples)
Limit of detection: 0.10 ng/g
Limit of quantification: 17.2 µg/g

See: http://www.chem.agilent.com/Library/applications/5990-5059EN.pdf

EPA test methods available for use in detecting the presence of mercury

Method 7471B (PDF) (7 pp, 111K)
Mercury in Solid or Semisolid Waste (Manual Cold-Vapor Technique)
The typical instrument detection limit (IDL) for this method is 0.0002 mg/L.

Method 7473 (PDF) (15 pp, 315K)
Mercury in Solids and Solutions by Thermal Decomposition, Amalgamation, and Atomic Absorption Spectrophotometry.
The instrument detection limit (IDL) for this method is 0.01 ng of total mercury.

http://www.epa.gov/osw/hazard/tsd/mercury/tests.htm

Sampling/Analytical methods in ambient air

NIOSH 6009 Mercury: http://www.cdc.gov/niosh/docs/2003-154/pdfs/6009.pdf

SOP to describe the procedures used to sample mercury vapor in ambient air using the Ohio Lumex RA-915 monitor.

http://www.renewnyc.com/content/pdfs/130liberty/SeptemberDeconstruction/B_SOP_for_OhioLumex.pdf

Appendix 11. Calculations (SEA)

Calculation of estimated changes in use over time for phenylmercury compounds
Use 10 years ago was 2-3 times greater than it is today.
Two scenarios: (1) remains at current levels and (2) continues to decline at an exponential rate, assuming use 10 years previously was 2.5 times current (= 2008 in Annex XV dossier).
Exponential decay function

k	0,092	(rate constant)		
t	X	Year	X	
0	100	1998	100,0	Value assumed to be 2.5 times greater than current use
1		1999	91,2	
2		2000	83,3	
3		2001	76,0	
4		2002	69,3	
5		2003	63,2	
6		2004	57,7	
7		2005	52,7	
8		2006	48,0	
9		2007	43,8	
10	40	2008	40,0	Values quoted in the draft Annex XV dossier
11		2009	36,5	
12		2010	33,3	
13		2011	30,4	
14		2012	27,7	End of this year, restriction is adopted
15		2013	25,3	
16		2014	23,1	End of this year is timescale for implementation for option 2
17		2015	21,1	
18		2016	19,2	
19		2017	17,5	End of this year is timescale for implementation for option 1
20		2018	16,0	
21		2019	14,6	
22		2020	13,3	
23		2021	12,2	
24		2022	11,1	
25		2023	10,1	
26		2024	9,2	
27		2025	8,4	
28		2026	7,7	
29		2027	7,0	
30		2028	6,4	
31		2029	5,8	
32		2030	5,3	
33		2031	4,9	
34		2032	4,4	
35		2033	4,0	
36		2034	3,7	

37	2035	3,4
38	2036	3,1
39	2037	2,8
40	2038	2,6
41	2039	2,3
42	2040	2,1

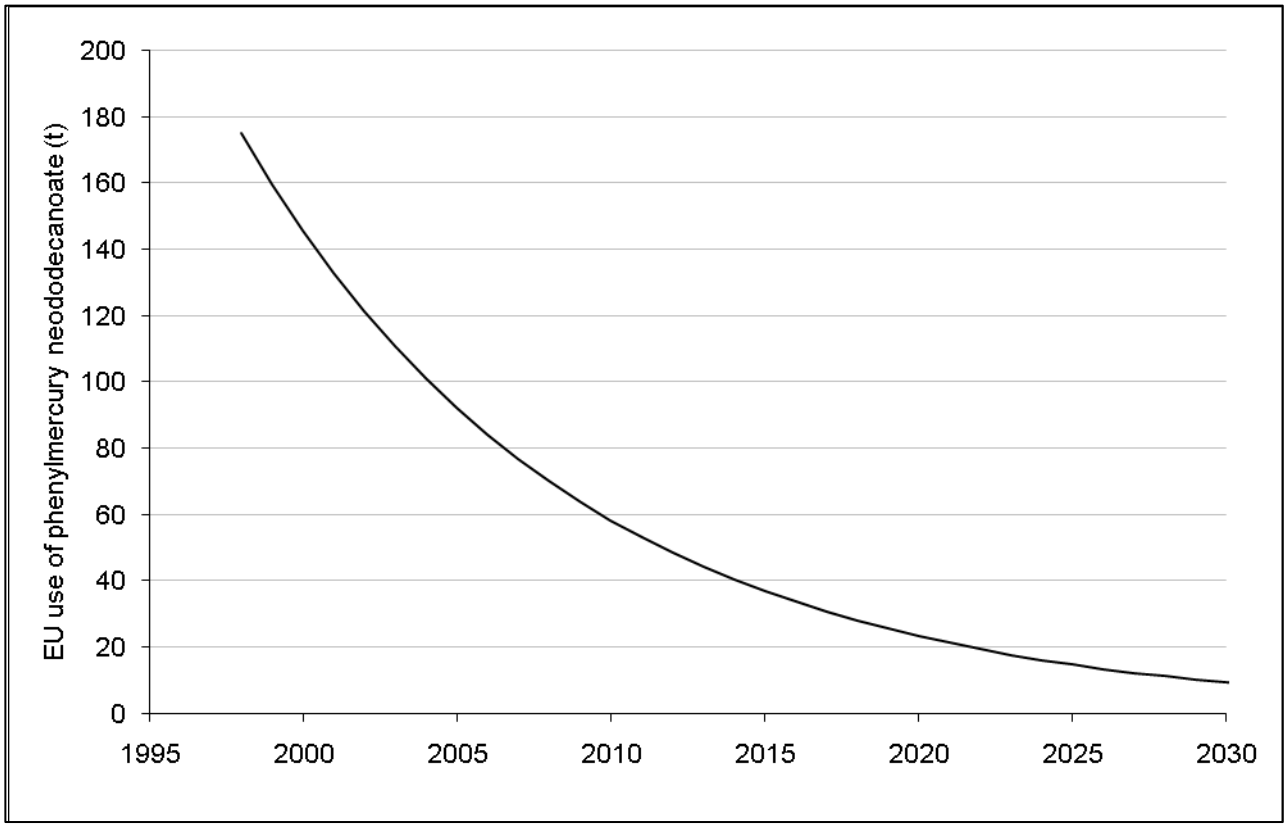
Estimated 2008 usage from table B.2.1 Annex XV dossier

	Phenylmercury acetate	Phenylmercury propionate	Phenylmercury 2-ethylhexanoate	Phenylmercuric octanoate	Phenylmercury neodecanoate
Production	5-10	~ 0	50-100	~ 0	75-150
Export	5-10	~ 0	49-99	~ 0	40 - 85
Import	<1	~ 0	~ 0	~ 0	< 5
For use in EU+EFTA	<1	~ 0	< 1	~ 0	36 - 70

Graphical representation for phenymercury neodecanoate
Scenario 1 = linear change with future use continuing at current levels
Scenario 2 = exponential decline in use
Plot shows usage over time, assuming high end of range is used.

2008	70	36	70	36	
1998	175	90	175	90	(2.5 times value in 2008)
Year	Scenario 1 High	Scenario 1 Low	Scenario 2 High	Scenario 2 Low	
1998	175	90	175	90	
1999	164,5	84,6	160	82	
2000	154	79,2	146	75	
2001	143,5	73,8	133	68	
2002	133	68,4	121	62	
2003	122,5	63	111	57	
2004	112	57,6	101	52	
2005	101,5	52,2	92	47	
2006	91	46,8	84	43	
2007	80,5	41,4	77	39	
2008	70	36	70	36	0,4
2009	70	36	64	33	
2010	70	36	58	30	
2011	70	36	53	27	
2012	70	36	49	25	
2013	70	36	44	23	
2014	70	36	40	21	
2015	70	36	37	19	
2016	70	36	34	17	
2017	70	36	31	16	
2018	70	36	28	14	0,4
2019	70	36	26	13	
2020	70	36	23	12	
2021	70	36	21	11	
2022	70	36	19	10	

2023	70	36	18	9
2024	70	36	16	8
2025	70	36	15	8
2026	70	36	13	7
2027	70	36	12	6
2028	70	36	11	6
2029	70	36	10	5
2030	70	36	9	5
2031	70	36	9	4
2032	70	36	8	4
2033	70	36	7	4
2034	70	36	6	3
2035	70	36	6	3
2036	70	36	5	3
2037	70	36	5	3
2038	70	36	4	2
2039	70	36	4	2
2040	70	36	4	2



	Phenylmercury acetate	Phenylmercury propionate	Phenylmercury 2-ethylhexanoate	Phenylmercuric octanoate	Phenylmercury neodecanoate
Fraction of Hg pr kg PhHg	0,596	0,572	0,477	0,477	0,447

Emission factors Life cycle stage	Air	Waste water	Soil	Total
Manufacturing	-	-	-	-
Formulation and processing	0,075	0,0006	0,00001	0,076
Service life	0,095	0,010	-	0,105
Waste incineration	0,100	0,0002	-	0,100
Landfilling	0,0005	-	-	0,001

Emissions estimates
Table B9.6 from Annex XV dossier (tonnes Hg/lifecycle stage) (2008 data)

Life cycle stage	Air	Waste water	Landfills
Manufacturing	-	-	n.d.
Formulation and processing	2,35	0,02	-
Service life	2,75	0,26	18,40
Waste incineration	0,75	0,00	6,76
Landfilling	0,25	-	-
Total emission	6,10	0,28	25,16

Estimated use of the different compounds, avoided through a restriction (tonnes).

Use avoided	Fraction of 2008 usage	Neodecanoate in the EU	Neodecanoate exported	2-ethylhexanoate exported	Acetate exported	Total use and production
Annual use in 2008, tonnes (PhHg)		70	85	99	10	264
Annual use in 2008, tonnes (Hg)		31	38	47	6	122
1996						
1997						
1998						
1999						
2000						
2001						
2002						
2003						
2004						
2005						
2006						
2007						
2008						
2009						
2010						
2011						
2012						
2013						
2014						
2015	0,53	16	20	25	3	64
2016	0,48	15	18	23	3	59
2017	0,44	14	17	21	3	54
2018	0,40	13	15	19	2	49
2019	0,36	11	14	17	2	45
2020	0,33	10	13	16	2	41
2021	0,30	10	12	14	2	37
2022	0,28	9	11	13	2	34
2023	0,25	8	10	12	2	31
2024	0,23	7	9	11	1	28
2025	0,21	7	8	10	1	26
2026	0,19	6	7	9	1	24
2027	0,18	5	7	8	1	21
2028	0,16	5	6	8	1	20
2029	0,15	5	6	7	1	18
2030	0,13	4	5	6	1	16
2031	0,12	4	5	6	1	15
2032	0,11	3	4	5	1	14
2033	0,10	3	4	5	1	12
2034	0,09	3	4	4	1	11
2035	0,08	3	3	4	1	10

2036	0,08	2	3	4	0	9
2037	0,07	2	3	3	0	9
2038	0,06	2	2	3	0	8
2039	0,06	2	2	3	0	7
2040	0,05	2	2	3	0	7
Total use avoided 2015-2024 (tonnes Hg)		113	137	170	22	442
Total use avoided 2018-2027 (tonnes Hg)		86	104	129	16	336

Baseline emissions, Neodecanoate

	Fraction of 2008 usage	Formulation and processing Annual emissions	Service life Emissions dependent on service life	Waste incineration Emissions only occur once products enter waste stream	Landfilling Emissions only occur once products enter waste stream. EF = 0.05% over 20 years.	Total emission
Annual emissions in 2008		2,36	3,01	0,75	0,25	6,38
1998	2,50					
1999	2,28					
2000	2,08					
2001	1,90					
2002	1,73					
2003	1,58					
2004	1,44					
2005	1,32					
2006	1,20					
2007	1,10					
2008	1,00	2,36	3,65	1,19	0,470	7,67
2009	0,91	2,16	3,33	1,09	0,487	7,06
2010	0,83	1,97	3,04	0,99	0,503	6,50
2011	0,76	1,80	2,77	0,90	0,517	5,99
2012	0,69	1,64	2,53	0,83	0,530	5,52
2013	0,63	1,50	2,31	0,75	0,543	5,10
2014	0,58	1,36	2,10	0,69	0,554	4,71
2015	0,53	1,24	1,92	0,63	0,565	4,36
2016	0,48	1,14	1,75	0,57	0,574	4,03
2017	0,44	1,04	1,60	0,52	0,583	3,74
2018	0,40	0,95	1,46	0,48	0,591	3,47
2019	0,36	0,86	1,33	0,43	0,598	3,23
2020	0,33	0,79	1,21	0,40	0,605	3,00
2021	0,30	0,72	1,11	0,36	0,611	2,80
2022	0,28	0,66	1,01	0,33	0,302	2,30
2023	0,25	0,60	0,92	0,30	0,275	2,10
2024	0,23	0,55	0,84	0,27	0,251	1,91
2025	0,21	0,50	0,77	0,25	0,229	1,75
2026	0,19	0,45	0,70	0,23	0,209	1,59
2027	0,18	0,41	0,64	0,21	0,191	1,45
2028	0,16	0,38	0,58	0,19	0,174	1,33
2029	0,15	0,35	0,53	0,17	0,159	1,21
2030	0,13	0,31	0,49	0,16	0,145	1,10

2031	0,12	0,29	0,44	0,14	0,132	1,01
2032	0,11	0,26	0,40	0,13	0,121	0,92
2033	0,10	0,24	0,37	0,12	0,110	0,84
2034	0,09	0,22	0,34	0,11	0,100	0,77
2035	0,08	0,20	0,31	0,10	0,092	0,70
2036	0,08	0,18	0,28	0,09	0,084	0,64
2037	0,07	0,17	0,26	0,08	0,076	0,58
2038	0,06	0,15	0,23	0,08	0,070	0,53
2039	0,06	0,14	0,21	0,07	0,064	0,48
2040	0,05	0,13	0,19	0,06	0,058	0,44
Total emission (2008-2040)		25,7	39,6	12,9	10,6	88,8

Mercury releases to the environment avoided in the EU through a restriction - emissions from year of restriction onwards (option 1) (tonnes)

Assumed average service life	5	years
Year of restriction entering into force	2018	
Fraction of 2008 usage in start year	0,40	

Formulation and processing: Emissions occur in the year in which use takes place. Based on 2008 emissions reduced by a factor
proportional to the use in the year in question.
Service life: Service life emissions are assumed to occur equally over the lifetime of the products.
In the first year, only emissions from
the first year's use are counted (one fifth), scaled according to use in that year
In the second year, emissions relate to one fifth of the use entering the market in the first year plus one fifth of those in the second year.
And so on until the sixth year when emissions relate to products entering the market in the 2nd to 6th years.
Waste incineration: Emissions occur only after the products enter the waste stream (i.e. there is a lag related to the service life of the products).
The emission in the start year +5 years relate to the 2008 emission scaled according to use in the start year.
Landfill: For each year's usage, emissions are 0.05% of the amount entering the waste stream
(If usage was steady at 2008 levels, emissions would be 0.05% x 27t x 20 years usage = 0.3t)
Emissions occur with a 5 year lag due to the assumed service life of the products.
For example, in year 2023, emissions are 1/20 of those related to use in 2018 (no previous years emissions are included because they
are not affected by the restriction)
Then in year 2024, emissions are 1/20 of those related to use in 2018 plus 1/20 of those related to use in 2019.
In all cases, emissions related to products entering the market before the start year are not included because they will not be affected by the restriction.

	Fraction of 2008 usage	Formulation & processing	Service life	Waste incineration	Landfilling	Total emission
		Annual emissions	Emissions dependent on service life	Emissions only occur once products enter waste stream	Emissions only occur once products enter waste stream. EF = 0.05% over 20 years.	
Annual		2,36	3,01	0,75	0,25	6,38

emissions in 2008						
1999						0,00
2000						0,00
2001						0,00
2002						0,00
2003						0,00
2004						0,00
2005						0,00
2006						0,00
2007						0,00
2008						0,00
2009						0,00
2010						0,00
2011						0,00
2012						0,00
2013						0,00
2014						0,00
2015						0,00
2016						0,00
2017						0,00
2018	0,40	0,95	0,24			1,19
2019	0,36	0,86	0,46			1,32
2020	0,33	0,79	0,66			1,45
2021	0,30	0,72	0,84			1,56
2022	0,28	0,66	1,01			1,67
2023	0,25	0,60	0,92	0,30	0,005	1,83
2024	0,23	0,55	0,84	0,27	0,010	1,67
2025	0,21	0,50	0,77	0,25	0,014	1,53
2026	0,19	0,45	0,70	0,23	0,018	1,40
2027	0,18	0,41	0,64	0,21	0,021	1,28
2028	0,16	0,38	0,58	0,19	0,024	1,18
2029	0,15	0,35	0,53	0,17	0,027	1,08
2030	0,13	0,31	0,49	0,16	0,030	0,99
2031	0,12	0,29	0,44	0,14	0,032	0,91
2032	0,11	0,26	0,40	0,13	0,034	0,83
2033	0,10	0,24	0,37	0,12	0,037	0,77
2034	0,09	0,22	0,34	0,11	0,038	0,70
2035	0,08	0,20	0,31	0,10	0,040	0,65
2036	0,08	0,18	0,28	0,09	0,042	0,60
2037	0,07	0,17	0,26	0,08	0,043	0,55
2038	0,06	0,15	0,23	0,08	0,044	0,51
2039	0,06	0,14	0,21	0,07	0,045	0,47
2040	0,05	0,13	0,19	0,06	0,046	0,43
Total emission avoided (2018-2027)		6,5	7,1	1,3	0,1	14,9
Average annual emission over assessment timescale						1,49

Mercury releases to the environment avoided in the EU through a restriction - emissions from year of restriction onwards (option 2) (tonnes)

Assumed average service life 5 years
Year of restriction entering into force 2015
Fraction of 2008 usage in start year 0,53
Approach is the same as for option 1, but with the restriction starting earlier.
Assuming only 70% of systems replaceable before 2018

	Fraction of 2008 usage	Formulation and processing Annual emissions	Service life Emissions dependent on service life	Waste incineration Emissions only occur once products enter waste stream	Landfilling Emissions only occur once products enter waste stream. EF = 0.05% over 20 years.	Total emission
Annual emissions in 2008		2,36	3,01	0,75	0,25	6,38
1996						0,00
1997						0,00
1998						0,00
1999						0,00
2000						0,00
2001						0,00
2002						0,00
2003						0,00
2004						0,00
2005						0,00
2006						0,00
2007						0,00
2008						0,00
2009						0,00
2010						0,00
2011						0,00
2012						0,00
2013						0,00
2014						0,00
2015	0,53	0,87	0,22			1,09
2016	0,48	0,80	0,42			1,22
2017	0,44	0,73	0,61			1,33
2018	0,40	0,95	0,85			1,80

2019	0,36	0,86	1,07			1,93
2020	0,33	0,79	1,05	0,28	0,005	2,12
2021	0,30	0,72	1,03	0,25	0,009	2,01
2022	0,28	0,66	1,01	0,23	0,013	1,91
2023	0,25	0,60	0,92	0,30	0,018	1,84
2024	0,23	0,55	0,84	0,27	0,022	1,68
2025	0,21	0,50	0,77	0,25	0,027	1,54
2026	0,19	0,45	0,70	0,23	0,030	1,41
2027	0,18	0,41	0,64	0,21	0,034	1,30
2028	0,16	0,38	0,58	0,19	0,037	1,19
2029	0,15	0,35	0,53	0,17	0,040	1,09
2030	0,13	0,31	0,49	0,16	0,043	1,00
2031	0,12	0,29	0,44	0,14	0,045	0,92
2032	0,11	0,26	0,40	0,13	0,047	0,85
2033	0,10	0,24	0,37	0,12	0,049	0,78
2034	0,09	0,22	0,34	0,11	0,051	0,72
2035	0,08	0,20	0,31	0,10	0,053	0,66
2036	0,08	0,18	0,28	0,09	0,054	0,61
2037	0,07	0,17	0,26	0,08	0,056	0,56
2038	0,06	0,15	0,23	0,08	0,057	0,52
2039	0,06	0,14	0,21	0,07	0,058	0,48
2040	0,05	0,13	0,19	0,06	0,055	0,44
Total emission avoided (2015-2024)		7,5	8,0	1,3	0,1	16,9
Average annual emission over assessment timescale					1,69	

Estimated emissions potentially avoided through a restriction on manufacture.

Emissions potentially avoided outside the EU option 1	Fraction of 2008 usage	Formulation & processing Annual emissions	Service life Emissions dependent on service life	Waste incineration Emissions only occur once products enter waste stream	Landfilling Emissions only occur once products enter waste stream. EF = 0.05% over 20 years.	Total emission
Annual emissions in 2008		6,89	8,85	2,19	0,73	18,67
1999						0,00
2000						0,00
2001						0,00
2002						0,00
2003						0,00
2004						0,00
2005						0,00
2006						0,00
2007						0,00
2008						0,00
2009						0,00
2010						0,00
2011						0,00
2012						0,00
2013						0,00
2014						0,00
2015						0,00
2016						0,00
2017						0,00
2018	0,40	2,76	0,71			3,47
2019	0,36	2,52	1,35			3,87
2020	0,33	2,30	1,94			4,24
2021	0,30	2,09	2,48			4,58
2022	0,28	1,91	2,97			4,88
2023	0,25	1,74	2,71	0,88	0,015	5,35
2024	0,23	1,59	2,47	0,80	0,028	4,89
2025	0,21	1,45	2,26	0,73	0,040	4,48
2026	0,19	1,32	2,06	0,67	0,051	4,10
2027	0,18	1,21	1,88	0,61	0,061	3,76
2028	0,16	1,10	1,72	0,55	0,071	3,44
2029	0,15	1,01	1,56	0,51	0,079	3,16
2030	0,13	0,92	1,43	0,46	0,087	2,89
2031	0,12	0,84	1,30	0,42	0,094	2,66
2032	0,11	0,76	1,19	0,38	0,100	2,44
2033	0,10	0,70	1,08	0,35	0,106	2,24

2034	0,09	0,64	0,99	0,32	0,112	2,06
2035	0,08	0,58	0,90	0,29	0,116	1,89
2036	0,08	0,53	0,82	0,27	0,121	1,74
2037	0,07	0,48	0,75	0,24	0,125	1,60
2038	0,06	0,44	0,69	0,22	0,129	1,48
2039	0,06	0,40	0,63	0,20	0,132	1,36
2040	0,05	0,37	0,57	0,18	0,135	1,26
Total emission avoided (2018-2027)		18,9	20,8	3,7	0,2	43,6
Average annual emission over assessment timescale					4,36	

Estimated emissions potentially avoided through a restriction on manufacture.

Emissions potentially avoided outside the EU option 2	Fraction of 2008 usage	Formulation and processing Annual emissions	Service life Emissions dependent on service life	Waste incineration Emissions only occur once products enter waste stream	Landfilling Emissions only occur once products enter waste stream. EF = 0.05% over 20 years.	Total emission
Annual emissions in 2008		6,89	8,85	2,19	0,73	18,67
1996						0,00
1997						0,00
1998						0,00
1999						0,00
2000						0,00
2001						0,00
2002						0,00
2003						0,00
2004						0,00
2005						0,00
2006						0,00
2007						0,00
2008						0,00
2009						0,00
2010						0,00
2011						0,00
2012						0,00
2013						0,00
2014						0,00
2015	0,53	2,54	0,65			3,19
2016	0,48	2,32	1,25			3,57
2017	0,44	2,12	1,79			3,91

2018	0,40	1,93	2,50			4,43
2019	0,36	1,76	3,14			4,91
2020	0,33	1,61	3,08	0,81	0,013	5,51
2021	0,30	1,47	3,02	0,74	0,026	5,25
2022	0,28	1,34	2,97	0,67	0,037	5,02
2023	0,25	1,22	2,71	0,88	0,052	4,86
2024	0,23	1,11	2,47	0,80	0,065	4,45
2025	0,21	1,02	2,26	0,73	0,078	4,08
2026	0,19	0,93	2,06	0,67	0,089	3,74
2027	0,18	0,85	1,88	0,61	0,099	3,43
2028	0,16	0,77	1,72	0,55	0,108	3,15
2029	0,15	0,70	1,56	0,51	0,117	2,89
2030	0,13	0,64	1,43	0,46	0,124	2,66
2031	0,12	0,59	1,30	0,42	0,131	2,44
2032	0,11	0,54	1,19	0,38	0,138	2,25
2033	0,10	0,49	1,08	0,35	0,144	2,07
2034	0,09	0,45	0,99	0,32	0,149	1,90
2035	0,08	0,41	0,90	0,29	0,154	1,76
2036	0,08	0,37	0,82	0,27	0,158	1,62
2037	0,07	0,34	0,75	0,24	0,162	1,50
2038	0,06	0,31	0,69	0,22	0,166	1,38
2039	0,06	0,28	0,63	0,20	0,170	1,28
2040	0,05	0,26	0,57	0,18	0,055	1,07
Total emission avoided (2015-2024)		17,4	23,6	3,9	0,2	45,1
Average annual emission over assessment timescale						4,51

Appendix 12. Theoretical studies of phenylmercury carboxylates

Appendix 13. EcetocTraWorkerTool calculations

Appendix 14. Break-even calculations, exported volumes