Substance name: 5-tert-butyl-2,4,6-trinitro-m-xylene
(musk xylene)
EC number: 201-329-4
CAS number: 81-15-2

PRIORITISATION AND ANNEX XIV BACKGROUND INFORMATION

14 January 2009
Disclaimer:

The present document has been developed by ECHA based on the information available from the “Proposal for identification of 5-tert-butyl-2,4,6-trinitro-m-xylene as a Substance of Very High Concern”, summarised in the respective support document (ECHA, 2008), the relevant Risk Assessment Report (EC, 2005) and further documents listed under references.

Note that the information on alternatives is not intended to be an exhaustive analysis, but is only included in order to support the transitional arrangements and in particular the proposed application dates for substances proposed to be included in Annex XIV.
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1 Prioritisation
Musk xylene is a vPvB and all its uses are wide dispersive, resulting in a nearly 100% release of the substance. Hence, although the volume used is presumably relatively low, it is proposed to prioritise 5-tert-butyl-2,4,6-trinitro-m-xylene (Musk xylene) for inclusion in Annex XIV.

2 Identity of the substance

Chemical name: Musk xylene
EC Number: 201-329-4
CAS Number: 81-15-2
IUPAC Name: 1-tert-butyl-3,5-dimethyl-2,4,6-trinitrobenzene

3 Intrinsic properties
The substance has been identified as a Substance of Very High Concern according to article 57(e) as it is identified as a vPvB substance as reported in the support document on Musk xylene and the agreement of the MSC adopted on 8 October 2008.

4 Volume(s)
The substance is not manufactured in the EU but imported as a pure substance from outside EU. The imported volume corresponds largely to the volume used within the EU as the export of the substance or the finished products out of the EU is considered to be minimal. The volume of uses was reported as 67 tonnes in 2000. However, a clear decrease has been observed since then (RPA, 2008). Within the time frame of the study no updated information became available on the actual imported volumes. A reasonable estimate of approximately 25 tonnes/year was extrapolated based on the decreasing trend from the past (22% decrease between 1998 and 2000). Furthermore, there is no detailed information about the presence of musk xylene in articles imported or exported. However, it is likely to be negligible as musk xylene is mainly used in preparations rather than articles.

In conclusion, no actual data on the volume of musk xylene used in the EU is available. Based on the decreasing trend observed in the recent past the volume currently used is estimated to approximately 25 tonnes/year.

5 Characterisation of uses and releases

5.1 Manufacture and uses
**Manufacture**

At present no manufacturing of musk xylene is taking place within the EU.

**Uses**

Musk xylene belongs to the family of synthetic musks which are substances used to emulate the aroma produced by natural musk. Musk ingredients are a significant ingredient for fragrance formulation both as fragrance and fragrance enhancers used in most fragrance mixtures for detergents, fabric softeners, fabric conditioners, cleaning agents, air fresheners and other household products (RPA, 2008).

It is assumed in the report (RPA, 2008) that 80% of the overall tonnage is used in detergents, cleaning products and fabric softeners and 20% of this tonnage is used in toiletries, colognes, shampoos, etc. This corresponds to 20 and 5 tonnes when taking into account the more reasonable estimate for the use volume (25 tonnes/year).

**5.2 Releases**

The number of EU relevant sites formulating and compounding of the substance is estimated at less than 10. The releases from these point sources are thought to be negligible compared to the overall diffuse releases coming from the use of consumer products containing the substance (EC, 2005).

The main releases come from the use by consumers of end products containing the substance. It is assumed (as a worst case) that 100% of the EU use volume is released into waste water and that no substance remains on the fabric, skin or surfaces or has evaporated. For detergents it is further assumed (RPA, 2008) that 75% of the musk xylene ends up in domestic wastewater while 25% ends up in industrial wastewater. For the private use of the substance and the regional scale it is considered that 20% of the releases go directly to the surface water whereas 80% go via a municipal Sewage Treatment Plant (STP). When in the STP it is assumed that 43% is discharged directly to the surface waters and 57% is adsorbed to sludge. This sludge can later on be incinerated, landfilled or spread on agricultural soil. Within the study, it is estimated that 25 tonnes/year is released into the environment (13 tonnes/year to water and 12 tonnes per year to sludge) (RPA, 2008).

**5.3 Geographical distribution**

There is no specific information regarding the geographical distribution of the different sites where the substance is compounded and formulated into preparations. The only information available is that the number of sites is rather small (<10 sites) (RPA, 2008).

There is no specific information regarding the use by consumers but as the end products are mainly for private use one can expect a wide distribution of the end products in the EU. The risk assessment report (EC, 2005) mentions that the
consumption is higher in southern countries than in northern countries. No update of these market characteristics could be obtained in the short term of the RPA study.

5.4 Conclusions on wide dispersiveness of uses

Musk xylenes are mainly used in preparations for consumer use such as e.g. detergents, cleaning products, fabric softeners as well as in toiletries, colognes and shampoos. It can be assumed that these uses occur widespread all over the EU and that they will result in nearly 100% release of the substance. Hence, these uses are wide-dispersive.

6 Complexity of the supply chain

Based on the information provided by the study (RPA, 2008) it can be concluded that:

1) the supply chain of this substance does not contain many levels (from the manufacturer/importer to the last actor affected by a possible authorisation decision).
2) the supply chain does not contain EU manufacturers but contains a high number of downstream (private) users.
3) the supply chain contains limited types of industry branches but producing a large number of different products. In addition, these industry branches are well organised in effective industry associations (cosmetics industry, detergents and cleaning products industry and fragrances formulators).

Furthermore, the available information has shown that the “self regulation” of musk xylene that has taken place during the last decade, has not drastically changed the supply chains compared to the previous market situation.

Therefore, it can be concluded that the supply chain for musk xylene is rather simple: the substance is imported, compounded into the fragrance (at less than 10 sites in the EU) and then formulated into a large number of end products mainly destined for consumer use.

7 Alternatives

Fragrances/perfumes are usually made up of top, middle and base notes. The base notes are usually the strongest scent and last longer than the top and middle notes (which are perceived shortly after application of the perfume). Base notes are, therefore, chosen because of their fixative properties, strength and/or scent. Musk xylene is one of a number of base notes which may be employed to ‘fix’ aromas in a range of consumer products.

Details on four main groups of synthetic musks (nitromusks, polycyclic musks, macrocyclic musks and alicyclic musks) which may, in theory, be considered to be alternatives to musk xylene (taking into account existing restrictions on their use in certain products, e.g. cosmetics) can be found in RPA (2008).
In discussing these alternatives, it is important to bear in mind that while, in theory, all the above synthetic musks possess what is often referred to as a “typical musky odour”, in practice, the odour profile for each compound is different and the resulting fragrance is a function of the manufacturing process as much as the type and quantity of musk compound used.

7.1 Human Health and Environmental Effects

Conclusion on the hazard profile of the alternatives

Details on the hazard properties of the alternative musk compounds can be found in RPA (2008). These data suggest that, currently, substitution in the market seems to be ongoing. However, at present important data gaps still exist to come to a conclusive answer on the hazardous properties for both the macrocyclic and alicyclic musks.

7.2 Technical and Economic Feasibility and Availability

In RPA (2008), the technical suitability of the different alternatives is discussed. The report indicates that, for example, the odour profiles (i.e. intensity, tonality, odour threshold, tenacity, etc) for macrocyclic musks are completely different from those for nitromusks and polycyclic musks. Kraft & Swift (2005) indicate that they differ technically from the other musks possessing superior odour characteristics; the company “Huber the Nose” (nd), however, indicates that this difference in odour profiles is the reason why some products still rely on fragrances containing nitromusks and polycyclic musks, even newly introduced ones. Macrocyclic musks are also less economic compared to the other musks. In fact, they were not commercially produced and commonly utilised until the late 1990s due to difficulties in their synthesis, relatively high cost of production and consequently higher price (and were consequently treated as trade secrets). Rowe (2004) notes that to replace or even outperform polycyclic musks and nitromusks in diverse applications, one can either lower the production price of macrocyclic musks or increase their odour intensity, which means lowering their odour threshold. The latter option allows for more complex synthetic approaches and accordingly higher production costs (Rowe, 2004).

Conclusion on the technical and economic feasibility and availability of the alternatives

The available alternatives appear to be technically suitable for the various end-products in which they are used, however, it is important to keep in mind the complexity of replacing an odour simply by replacing a single substance. In practice, the odour profile for each compound is different and the resulting fragrance is a function of the manufacturing process as much as the type and quantity of musk compound used.

Regarding the economic feasibility of substitutes, it is clear that although macrocyclic musks appear to be more costly compared to musk xylene (and other musks), some companies have already incurred these costs in any case.
8  Existing Community legislation relevant for possible exemptions

No data available

9  Other information

No data available

10 References


Huber the Nose (nd): *Interesting Facts in Our Field, Passion for Scents*, by Huber the Nose. Article downloaded from the Huber the Nose Company website: [www.thenose.ch/files/htn_musks.pdf](http://www.thenose.ch/files/htn_musks.pdf)

