

1

2

3 **Guidance on**

4 **information requirements and chemical safety assessment**

5 **Chapter R.7a: Endpoint specific guidance**

6

7 **FIRST DRAFT FOR PEG**

8 **2nd March 2012**

9

10

11

12 **Guidance for the implementation of REACH**

13

14

15

16

17

18

19

20

21

22

23

24

25

26

27

28

29

30

31

32

33

34 **Version 2**

35

36 **Xxxx 2012**

LEGAL NOTICE

This document contains guidance on REACH explaining the REACH obligations and how to fulfil them. However, users are reminded that the text of the REACH Regulation is the only authentic legal reference and that the information in this document does not constitute legal advice. The European Chemicals Agency does not accept any liability with regard to the contents of this document.

Guidance on information requirements and chemical safety assessment

Chapter R.7a: Endpoint specific guidance

Reference:
Publ.date: xxxx 2012
Language: EN

© European Chemicals Agency, 2012

Cover page © European Chemicals Agency

Reproduction is authorised provided the source is fully acknowledged in the form “Source: European Chemicals Agency, <http://echa.europa.eu/web/guest>”, and provided written notification is given to the ECHA Communication Unit (publications@echa.europa.eu).

If you have questions or comments in relation to this document please send them (indicating the document reference, issue date, chapter and/or page of the document which your comment refers to) using the Guidance feedback form. The feedback form can be accessed via the ECHA Guidance website or directly via the following link:

https://comments.echa.europa.eu/comments_cms/FeedbackGuidance.aspx

European Chemicals Agency

Mailing address: P.O. Box 400, FI-00121 Helsinki, Finland

Visiting address: Annankatu 18, Helsinki, Finland

PREFACE

This document describes the information requirements under REACH with regard to substance properties, exposure, uses and risk management measures, and the chemical safety assessment. It is part of a series of guidance documents that are aimed to help all stakeholders with their preparation for fulfilling their obligations under the REACH regulation. These documents cover detailed guidance for a range of essential REACH processes as well as for some specific scientific and/or technical methods that industry or authorities need to make use of under REACH.

The guidance documents were drafted and discussed within the REACH Implementation Projects (RIPs) led by the European Commission services, involving stakeholders from Member States, industry and non-governmental organisations. After acceptance by the Member States Competent Authorities the guidance documents had been handed over to ECHA for publication and further maintenance. Any updates of the guidance are drafted by ECHA and are then subject to a consultation procedure, involving stakeholders from Member States, industry and non-governmental organisations. For details of the consultation procedure, please see:

http://echa.europa.eu/documents/10162/17203/mb_14_2011_consultation_procedure_guidance_en.pdf

The guidance documents can be obtained via the website of the European Chemicals Agency

<http://echa.europa.eu/web/guest/guidance-documents/guidance-on-reach>

Further guidance documents will be published on this website when they are finalised or updated.

This document relates to the REACH Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006¹.

¹ Corrigendum to Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), establishing a European Chemicals Agency, amending Directive 1999/45/EC and repealing Council Regulation (EEC) No 793/93 and Commission Regulation (EC) No 1488/94 as well as Council Directive 76/769/EEC and Commission Directives 91/155/EEC, 93/67/EEC, 93/105/EC and 2000/21/EC (OJ L 396, 30.12.2006); amended by amended by: Council Regulation (EC) No 1354/2007 of 15 November 2007 adapting Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH), by reason of the accession of Bulgaria and Romania, Commission Regulation (EC) No 987/2008 of 8 October 2008 as regards Annexes IV and V; Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures; Commission regulation No 453/2010 of 20 May 2010 as regards Annex II; Commission Regulation No 252/2011 of 15 March 2011 as regards Annex I; Commission Regulation No 366/2011 of 14 April as regards Annex XVII (Acrylamide), Commission Regulation No 494/2011 of 20 May 2011, as regards Annex XVII (Cadmium).

Document Histroy

Version	Comment	Date
Version 1	First edition	May 2008
Version 2		Xxxx 2012

Convention for citing the REACH and the CLP Regulations

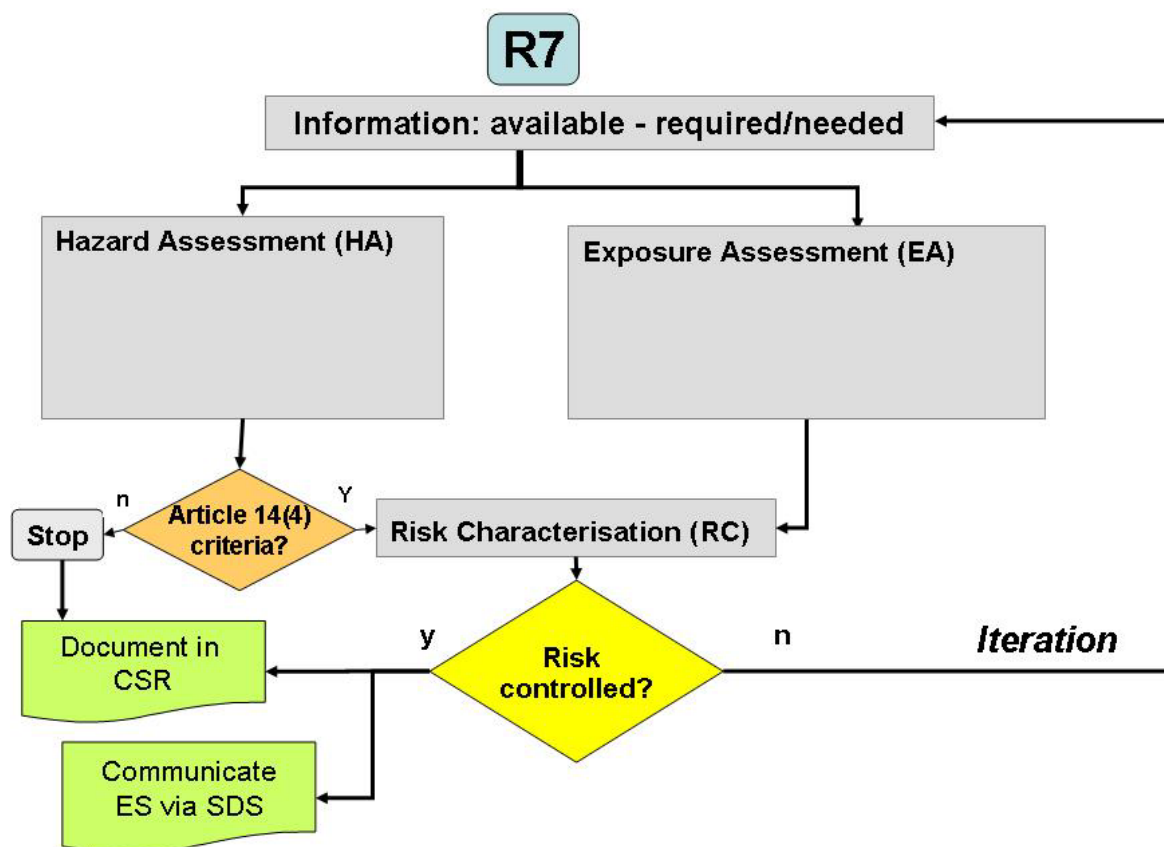
Where the REACH and the CLP Regulations are cited literally, this is indicated by text in italics between quotes.

Table of Terms and Abbreviations

See Chapter R.20

Pathfinder

The figure below indicates the location of part R.7(a) within the Guidance Document



- 1
- 2

CONTENTS

TABLE OF CONTENTS

R.7	ENDPOINT SPECIFIC GUIDANCE	13
Introduction		13
Information requirements in the light of the applicable classification regime		15
Use of data derived from EU or other international standardised test methods.....		15
Interdependence of endpoints in hazard assessment.....		16
Adequacy of methods for generating additional information		16
Degradation products and metabolites		17
Selection of the appropriate route of exposure for toxicity testing.....		18
R.7.1 Physico-chemical properties		19
R.7.1.1 Introduction.....		19
R.7.1.1.1 Information requirements on physico-chemical properties		19
R.7.1.1.2 Available information on physico-chemical properties.....		23
R.7.1.1.3 Evaluation of available information on physico-chemical properties		23
Experimental data		23
Non-experimental data		24
Uncertainty evaluation of data.....		24
Quality assurance for the determination of physico-chemical properties.....		24
Use of secondary and historical data sources for physico-chemical properties.....		24
Assessing the quality of QSPR models		25
R.7.1.1.4 General testing strategy for physico-chemical properties/hazards		26
R.7.1.1.5 Overall consistency of the physico-chemical profile.....		31
R.7.1.1.6 References for introduction of Physico-Chemical properties.....		35
R.7.1.2 MELTING/FREEZING POINT		36
R.7.1.2.1 Type of property		36
R.7.1.2.2 Definition		36
R.7.1.2.3 Test method(s).....		36
R.7.1.2.4 Adaptation of the standard testing regime.....		36
Waiving possibilities according to column 2 of Annex VII to REACH.....		36
Waiving possibilities according to Annex XI to REACH		37
Further waiving possibilities		37
R.7.1.2.5 Impurities; uncertainties		37
R.7.1.2.6 Endpoint specific information in the registration dossier/ IUCLID		37
R.7.1.3 BOILING POINT		38
R.7.1.3.1 Type of property		38
R.7.1.3.2 Definition		38
R.7.1.3.3 Test method(s).....		38
R.7.1.3.4 Adaptation of the standard testing regime.....		39
Waiving possibilities according to column 2 of Annex VII to REACH.....		39
Waiving possibilities according to Annex XI to REACH		39
Further waiving possibilities		40
R.7.1.3.5 Impurities; uncertainties		40
R.7.1.3.6 Endpoint specific information in the registration dossier / in IUCLID		40
R.7.1.4 RELATIVE DENSITY		41
R.7.1.4.1 Type of property		41
R.7.1.4.2 Definition		41
R.7.1.4.3 Test method(s).....		41
Adaptation of the standard testing regime		42
R.7.1.4.4		42
Waiving possibilities according to column 2 of Annex VII to REACH.....		42
Waiving possibilities according to Annex XI to REACH		42

1	Further waiving possibilities	43
2	R.7.1.4.5 Impurities; uncertainties	43
3	R.7.1.4.6 Endpoint specific information in the registration dossier / in IUCLID	43
4	R.7.1.5 VAPOUR PRESSURE	45
5	R.7.1.5.1 Type of property	45
6	R.7.1.5.2 Definition	45
7	R.7.1.5.3 Test method(s)	45
8	R.7.1.5.4 Adaptation of the standard testing regime	45
9	Waiving possibilities according to column 2 of Annex VII to REACH	45
10	Waiving possibilities according to Annex XI to REACH	46
11	Further waiving possibilities	48
12	R.7.1.5.5 Impurities; uncertainties	48
13	R.7.1.5.6 Endpoint specific information in the registration dossier / in IUCLID	49
14	References on vapour pressure	50
15	R.7.1.5.7	50
16	R.7.1.6 SURFACE TENSION	51
17	R.7.1.6.1 Type of property	51
18	R.7.1.6.2 Definition	51
19	R.7.1.6.3 Test method(s)	51
20	R.7.1.6.4 Adaptation of the standard testing regime	51
21	Waiving possibilities according to column 2 of Annex VII to REACH	51
22	Waiving possibilities according to Annex XI to REACH	52
23	Further waiving possibilities	53
24	R.7.1.6.5 Impurities; uncertainties	53
25	R.7.1.6.6 Endpoint specific information in the registration dossier / in IUCLID	53
26	R.7.1.6.7 References on surface tension	54
27	R.7.1.7 WATER SOLUBILITY	56
28	R.7.1.7.1 Type of property	56
29	R.7.1.7.2 Definition	56
30	R.7.1.7.3 Test method(s)	57
31	Adaptation of the standard testing regime	58
32	R.7.1.7.4	58
33	Waiving possibilities according to column 2 of Annex VII to REACH	58
34	Waiving possibilities according to Annex XI to REACH	59
35	Further waiving possibilities	61
36	R.7.1.7.5 Impurities; uncertainties	61
37	R.7.1.7.6 Endpoint specific information in the registration dossier / in IUCLID	61
38	R.7.1.7.7 References on water solubility	63
39	R.7.1.8 PARTITION COEFFICIENT <i>n</i> -OCTANOL/WATER	64
40	R.7.1.8.1 Type of property	64
41	R.7.1.8.2 Definition	64
42	R.7.1.8.3 Test method(s)	64
43	R.7.1.8.4 Adaptation of the standard testing regime	66
44	Waiving possibilities according to column 2 of Annex VII to REACH	67
45	Waiving possibilities according to Annex XI to REACH	67
46	Further waiving possibilities	69
47	R.7.1.8.5 Impurities; uncertainties	69
48	R.7.1.8.6 Endpoint specific information in the registration dossier / in IUCLID	70
49	R.7.1.8.7 References on <i>n</i> -octanol/water partition coefficient	72
50	R.7.1.9 FLASH POINT	74
51	R.7.1.9.1 Type of property	74
52	R.7.1.9.2 Definition	74
53	R.7.1.9.3 Test method(s)	74
54	R.7.1.9.4 Adaptation of the standard testing regime	74
55	Waiving possibilities according to column 2 of Annex VII to REACH	74
56	Waiving possibilities according to Annex XI to REACH	75
57	Further waiving possibilities	75
58	R.7.1.9.5 Impurities; uncertainties	76
59	R.7.1.9.2 Endpoint specific information in the registration dossier / in IUCLID	76
60	R.7.1.10 FLAMMABILITY	77

1	R.7.1.10.1	Flammable gases	78
2	Definition	78	
3	Classification criteria and relevant information	78	
4	Adaptation of the standard testing regime	78	
5	Impurities; uncertainties	79	
6	How to conclude on the DSD classification	79	
7	Endpoint specific information in the registration dossier/in IUCLID	80	
8	Further information / references	80	
9	R.7.1.10.2	Flammable aerosols	80
10	R.7.1.10.3	Flammable liquids	80
11	Definition	80	
12	Classification criteria and relevant information	80	
13	Adaptation of the standard testing regime	81	
14	Impurities; uncertainties	83	
15	How to conclude on the DSD classification	83	
16	Endpoint specific information in the registration dossier/in IUCLID	84	
17	Further information / references	84	
18	R.7.1.10.4	Flammable solids	84
19	Definition	84	
20	Classification criteria and relevant information	85	
21	Adaptation of the standard testing regime	85	
22	Impurities; uncertainties	86	
23	How to conclude on the DSD classification	86	
24	Endpoint specific information in the registration dossier/in IUCLID	86	
25	Further information / references	87	
26	R.7.1.10.5	Self-reactive substances and mixtures	87
27	Definition	87	
28	Classification criteria and relevant information	87	
29	Adaptation of the standard testing regime	88	
30	Impurities; uncertainties	89	
31	How to conclude on the DSD classification	89	
32	What information is required in the registration dossier in IUCLID	89	
33	Further information / references	90	
34	R.7.1.10.6	Pyrophoric liquids	90
35	Definition	90	
36	Classification criteria and relevant information	90	
37	Adaptation of the standard testing regime	90	
38	Impurities; uncertainties	91	
39	How to conclude on the DSD classification	91	
40	Endpoint specific information in the registration dossier IUCLID	92	
41	Further information / references	92	
42	R.7.1.10.7	Pyrophoric solids	92
43	Definition	92	
44	Classification criteria and relevant information	92	
45	Adaptation of the standard testing regime	93	
46	Impurities; uncertainties	94	
47	How to conclude on the DSD classification	94	
48	Endpoint specific information in the registration dossier/in IUCLID	94	
49	Further information / references	94	
50	R.7.1.10.8	Self-heating substances and mixtures	94
51	Definition	94	
52	Classification criteria and relevant information	95	
53	Adaptation of the standard testing regime	95	
54	Impurities; uncertainties	96	
55	How to conclude on the DSD classification	96	
56	Endpoint specific information in the registration dossier/in IUCLID	96	
57	Further information / references	97	
58	R.7.1.10.9	Substances which in contact with water emit flammable gases	97
59	Definition	97	
60	Classification criteria and relevant information	97	

1	Adaptation of the standard testing regime	98
2	Impurities; uncertainties	99
3	How to conclude on the DSD classification	100
4	Endpoint specific information in the registration dossier/in IUCLID	100
5	Further information / references	100
6	R.7.1.10.10 Organic peroxides	100
7	Definition	100
8	Classification criteria and relevant information	101
9	Adaptation of the standard testing regime	101
10	Impurities; uncertainties	102
11	How to conclude on the DSD classification	102
12	Endpoint specific information in the registration dossier/in IUCLID	103
13	Further information / references	103
14	R.7.1.11 EXPLOSIVE PROPERTIES	104
15	R.7.1.11.1 Explosives	105
16	Definition	105
17	Classification criteria and relevant information	105
18	Adaptation of the standard testing regime	106
19	Impurities; uncertainties	108
20	How to conclude on the DSD classification	108
21	Endpoint specific information in the registration dossier/in IUCLID	109
22	Further information / references	109
23	R.7.1.11.2 Self-reactive substances and mixtures	110
24	Definition	110
25	Classification criteria and relevant information	110
26	Adaptation of the standard testing regime	110
27	Impurities; uncertainties	111
28	How to conclude on the DSD classification	111
29	What information is required in the registration dossier in IUCLID	111
30	Further information / references	112
31	R.7.1.11.3 Organic peroxides	112
32	Definition	112
33	Classification criteria and relevant information	113
34	Adaptation of the standard testing regime	113
35	Impurities; uncertainties	114
36	How to conclude on the DSD classification	114
37	Endpoint specific information in the registration dossier/in IUCLID	115
38	Further information / references	115
39	R.7.1.12 SELF-IGNITION TEMPERATURE	116
40	R.7.1.12.1 Auto- ignition	116
41	Type of property	116
42	Definition	117
43	Test method(s)	117
44	Adaptation of the standard testing regime	117
45	Impurities; uncertainties	118
46	Endpoint specific information in the registration dossier / in IUCLID	118
47	R.7.1.12.2 Self-heating substances	119
48	R.7.1.13 OXIDISING PROPERTIES	119
49	R.7.1.13.1 Oxidising gases	120
50	Definition	120
51	Classification criteria and relevant information	120
52	Adaptation of the standard testing regime	120
53	Impurities; uncertainties	122
54	How to conclude on the DSD classification	122
55	Endpoint specific information in the registration dossier/in IUCLID	122
56	Further information / references	122
57	R.7.1.13.2 Oxidising liquids	123
58	Definition	123
59	Classification criteria and relevant information	123
60	Adaptation of the standard testing regime	123

1	Impurities; uncertainties	125
2	How to conclude on the DSD classification	125
3	Endpoint specific information in the registration dossier/in IUCLID	125
4	Further information / references	126
5	R.7.1.13.3 Oxidising solids.....	126
6	Definition	126
7	Classification criteria and relevant information	126
8	Adaptation of the standard testing regime	127
9	Impurities; uncertainties	129
10	How to conclude on the DSD classification	129
11	Endpoints specific information in the registration dossier/in IUCLID	129
12	Further information / references	130
13	R.7.1.14 GRANULOMETRY	130
14	R.7.1.14.1 Type of property	130
15	R.7.1.14.2 Definitions.....	131
16	R.7.1.14.3 Test methods	132
17	R.7.1.14.4 Adaptation of the standard testing regime.....	140
18	Waiving possibilities according to column 2 of Annex VII to REACH.....	140
19	Waiving possibilities according to Annex XI to REACH	140
20	Further waiving possibilities	141
21	R.7.1.14.5 Impurities; uncertainties	141
22	R.7.1.14.6 Endpoint specific information in the registration dossier / in IUCLID	141
23	R.7.1.14.7 Further information / references	142
24	R.7.1.15 ADSORPTION/DESORPTION	143
25	R.7.1.15.1 Type of property	143
26	R.7.1.15.2 Definition	143
27	R.7.1.15.3 Test method(s).....	143
28	R.7.1.15.4 Adaptation of the standard testing regime.....	145
29	Waiving possibilities according to column 2 of Annex VII to REACH.....	145
30	Waiving possibilities according to Annex XI to REACH	146
31	Further waiving possibilities	147
32	R.7.1.15.5 Impurities;uncertainties	148
33	R.7.1.15.6 Endpoint specific information in the registration dossier/ in IUCLID	148
34	R.7.1.15.7 Further information/references.....	151
35	R.7.1.16 STABILITY IN ORGANIC SOLVENTS AND IDENTITY OF RELEVANT DEGRADATION	
36	PRODUCTS.....	152
37	R.7.1.16.1 Type of property	152
38	R.7.1.16.2 Definition	152
39	R.7.1.16.3 Test method(s).....	153
40	R.7.1.16.4 Adaptation of the standard testing regime.....	154
41	Waiving possibilities according to column 2 of Annex IX to REACH	154
42	Waiving possibilities according to Annex XI to REACH	154
43	Further waiving possibilities	154
44	R.7.1.16.5 Impurities; uncertainties	154
45	R.7.1.16.6 Endpoint specific information in the registration dossier / in IUCLID	154
46	R.7.1.16.7 Further information / references	155
47	R.7.1.17 DISSOCIATION CONSTANT	155
48	R.7.1.17.1 Type of property	155
49	R.7.1.17.2 Definition	156
50	R.7.1.17.3 Test method(s).....	157
51	R.7.1.17.4 Adaptation of the standard testing regime.....	157
52	Waiving possibilities according to column 2 of Annex IX to REACH	157
53	Waiving possibilities according to Annex XI to REACH	159
54	Further waiving possibilities	160
55	R.7.1.17.5 Impurities; uncertainties	160
56	R.7.1.17.6 Endpoint specific information in the registration dossier / in IUCLID	161
57	R.7.1.17.7 References on dissociation constant	162
58	R.7.1.18 VISCOSITY	163
59	R.7.1.18.1 Type of property	163
60	R.7.1.18.2 Definition	163

1	R.7.1.18.3	Test method(s).....	163
2	R.7.1.18.4	Adaptation of the standart testing regime.....	164
3		Waiving possibilities according to column 2 of Annex IX to REACH.....	164
4		Waiving possibilities according to Annex XI to REACH.....	164
5		Further waiving possibilities	165
6	R.7.1.18.5	Impurities; uncertainties	165
7	R.7.1.18.6	Endpoint specific information in the registration dossier / in IUCLID	165
8	R.7.1.19	PARAMETERS ONLY APPEARING IN THE CLP REGULATION	165
9	R.7.1.19.1	Gases under pressure.....	166
10	R.7.1.19.2	Corrosive to metals.....	166
11	R.7.2	Skin- and eye irritation/corrosion and respiratory irritation.....	167
12	R.7.2.1	Introduction.....	167
13			
14			
15			

R.7 ENDPOINT SPECIFIC GUIDANCE

Introduction

The previous sections of the Guidance on information requirements and chemical safety assessment (IR/CSA) provide advice on the interpretation and application of generic aspects of the Regulation describing the overall process that should be followed in finding, assembling and evaluating all the relevant information that is required for the registration of a chemical under the REACH Regulation (EC) No 1907/2006. The chapters also describe factors that may have an influence on the information requirements and give advice on how the information collected from different sources could be integrated and used in a *weight of evidence* (WoE) approach to allow a conclusion on whether or not the available information is sufficient for regulatory purposes, i.e. hazard assessment and risk assessment.

The guidance given thus far is applicable across the field and comprises the general rules that should be followed.

In this chapter, specific guidance on meeting the information requirements set out in Annexes VI to XI to the REACH Regulation is provided. The information requirements relate both to those physico-chemical properties that are relevant for exposure and fate considerations as well as to physical hazards, human health hazards and environmental hazards. The guidance for each specified property or hazard has been developed as a specific sub-chapter in this guidance, addressing the aspects of collection, generation and evaluation of information to help registrants provide adequate and relevant information for registration under REACH.

All data sources, including non-testing data have to be taken into account when doing the chemical safety assessment. Most of the reports follow a logical common format that complements the generic guidance and the general decision making frameworks detailed in first paragraph above. The first chapter, namely the R.7.1 Physico-chemical properties and physical hazards underwent a guidance revision process between 2011 and 2012 and therefore follows a revised chapter structure. The R.7.1 chapter covers both classification and non-classification related properties, where the sub-chapters covering the physico-chemical properties have each six or seven sections, depending on the need for information on references and the sub-chapters covering the physical hazards have seven sections. In the physico-chemical properties sub-chapters the first section details the type of property, the second section provides the definition of the property, the third lists the preferred test method(s). The fourth section deals with adaptation of the standard testing regime, namely waiving options that can be explored under each specific physico-chemical property. The fifth section deals with impurities and uncertainties and the last section outlines what kind of property-specific information should be given in the registration dossier and in IUCLID. Note that sometimes an additional section is added where relevant references are provided. By contrast the physical hazard sub-chapters start with the definition section, followed by a second section on classification criteria and relevant information. The third section explores various waiving options, namely how the standard testing regime can be adapted. The fourth section outlines the impurities and uncertainties. The fifth section aims to help in concluding on the Dangerous Substances Directive (DSD Directive 67/548/EEC) classification and the sixth section outlines the physical hazards-specific information to be included in the registration dossier and in IUCLID. The seventh section gives relevant further information and used references.

1 Chapters tackling human health properties or hazards in R.7(a) remain unchanged. In those
2 chapters there are six main sections to the guidance on each property or hazard; the
3 introduction section provides an introduction in which the property or hazard is described,
4 defined and an explanation given of its importance in the context of human health or
5 environmental fate and effect of a given substance. The first section details the specific
6 information requirements for the endpoint of interest; these will depend on the tonnage band
7 of the substance, its usage pattern and other considerations including data on other endpoints
8 and on related substances. Endpoint² specific guidance can be thought of as the four logical
9 steps that should be taken to assemble the information that is detailed under the second
10 section; thus, the second section provides an inventory of all the types of data that could
11 potentially provide useful information on the endpoint of interest and, most importantly the
12 sources of that information.

13 Guidance is given in the third section on how to evaluate the information that might be
14 available for a given substance; this advice focuses on providing the criteria to aid in the
15 judgement and ranking of the available data for their adequacy and completeness. This section
16 also provides an indication of the remaining uncertainty inherent in the different types of data
17 for the given endpoint.

18 The fourth section describes how conclusions may be drawn for a given substance on the
19 suitability of the available information for regulatory purposes. Guidance is given on how to
20 develop and apply a WoE approach for the endpoint in order to establish whether there is a
21 need for further information and if so, what test should be performed. Chemical safety
22 assessment within REACH is fundamentally dependent on an adequate conclusion on
23 classification and PBT/vPvB assessment since exposure assessment and risk characterisation
24 are triggered by classification and fulfilment of PBT/vPvB criteria. Therefore data need to be
25 adequate for both classification & labelling and for chemical safety assessment if the latter is
26 required.

27 The fifth section comprises an Integrated Testing Strategy (ITS) for the given endpoint(s),
28 providing guidance on how to define and generate relevant information on substances in order
29 to meet the requirements of REACH. It is noteworthy that all experiments using vertebrate
30 animals shall be designed to avoid distress and unnecessary pain and suffering to
31 experimental animals, in accordance to Article 7.4 of Directive 86/609/EEC.

32 The proposed testing strategies are guidance for data generation in a stepwise approach. The
33 strategies build on the concept that if the available information is not sufficient to meet the
34 regulatory needs, further gathering of information at a succeeding step in the testing strategies
35 is needed. On the other hand, if the available information is adequate and the standard
36 information requirements are met, no further gathering of information is necessary. In those
37 cases where the available information is judged to be sufficient to meet the regulatory needs
38 even though the standard information requirements are not met, under certain circumstances,

² REACH uses the term “endpoint” both to denote a physico-chemical property (example: Annex VII to REACH, Column 1 standard information required: 7.3 Boiling point, and 7.4 Relative density) and to denote hazardous properties (example: Annex VII to REACH, Column 1 standard information required: 7.11 Explosive properties and 7.13 Oxidising properties) which are subject to classification according to the applicable EU legislation. In the following, the wording of Part 7(a) of this guidance document will differentiate between these different types of properties where this appears appropriate, in order to facilitate the identification of properties which serve the regulatory purpose of classification.

in particular for Annexes IX and X to REACH, this might be part of a justification for waiving a certain test that is requested in the standard information requirements.

The final section lists all used references on the given endpoints.

The following additional considerations apply generally to the endpoint specific guidance given in this chapter:

Information requirements in the light of the applicable classification regime

The main regulatory purpose of the information requirements set out in Annexes VI to XI to REACH is to assess risks related to substances and to develop and recommend appropriate risk management measures, as highlighted in Recital 19 REACH. According to Recital 26: *‘in order to undertake chemical safety assessment of substances effectively, manufacturer and importers of substances should obtain information on these substances, if necessary by performing new tests’*. The chemical safety assessment (CSA) should be performed in accordance with the provisions set out in Annex I REACH. According to Section 0.6 of Annex I, the first three steps of the CSA require the carrying out of human health hazard assessment, human health hazard assessment of physicochemical properties and environmental hazard assessment, including determining the classification of substances. When the REACH Regulation was adopted, the DSD was the applicable classification regime (see, more in particular, the transitional provisions set out in Article 61 CLP). Accordingly, many REACH information requirements are inspired by the categories of danger under DSD such as points 7.10, 7.11 and 7.13 in column I of Annex VII to REACH (*i.e* flammability, explosive properties and oxidising properties).

On 20 January 2009 Regulation (EC) No 1272/2008 (CLP Regulation or CLP) entered into force. The CLP Regulation has amended certain parts of REACH (see Article 58 CLP for amendments applicable from 1st December 2010 and Article 59 CLP for amendments applicable from 1st June 2015), therefore the terminology used in REACH currently comprises terms which were still used under the DSD and still apply under the Dangerous Preparations Directive (DPD 1999/45/EC). With respect to the updated physico-chemical part of this guidance and the section dealing with the exploration of waiving possibilities/ adaptation of the standard testing regime, the term ‘dangerous’ can be interpreted in a broader context as it does not refer strictly to the DSD.

According to sections 4.1, 4.2 and 4.3 of Annex VI to REACH, as amended by Article 58(11) CLP, registrants have to provide in their registration dossiers the hazard classification of the substance(s) in accordance with Title I and II of CLP. Also, the provision of DSD classifications has no longer been required in the registration dossier since 1 December 2010. Nevertheless, under the transitional regime set out in Art. 61 CLP, DSD classifications are still applied until 1 June 2015 for the compilation of Safety Data Sheets (see Commission Regulation (EU) No 453/2010) and for the purposes of CLP itself (Article 61 (3) CLP).

Use of data derived from EU or other international standardised test methods

According to Article 13 (3) REACH, tests for generating information on intrinsic properties of substances shall be conducted in accordance with the test methods laid down in a Commission Regulation or according to other international test methods recognised by the Commission or the Agency as being appropriate, such as European international standards (www.cen.eu) or the OECD guidelines (www.oecd.org). Council Regulation (EC) 440/2008

(Test Method Regulation)³ lays down the test methods to be applied for the purposes of REACH. Other internationally standardised test methods are recognised by the Commission or the Agency as being adequate for generating data for regulatory use, thus, in the following sections on specific endpoints, references given for each test method will include the OECD Test Guideline (TG) number and, where available, the test method (A) number, as defined in the Test Method Regulation.

Toxicological and ecotoxicological tests and analyses shall be carried out in compliance with the principles of GLP. Studies must be conducted in accordance with the EU test methods laid down in Test Method Regulation or with other international test methods validated according to international procedures, such as those of the OECD.

According to Recital 37 REACH, if tests are performed, they should comply with the relevant requirements of protection of laboratory animals, set out in Council Directive 86/609/EEC⁴. Art. 13 (4) REACH states that ecotoxicological and toxicological tests and analyses shall be carried out in compliance with the principles of GLP provided for in Directive 2004/10/EC⁵ or other international standards recognised as being equivalent by the Commission or the Agency and with the provisions of Council Directive 86/609/EEC, if applicable. Under Art. 8 (5) CLP, where new test for physical hazards must be carried out for classification and labelling purposes, they must be performed in compliance with a relevant recognised quality system (e.g. GLP) or by laboratories complying with a relevant recognised standard (e.g. with EN ISO/IEC 17025), at the latest from January 2014.

Interdependence of endpoints in hazard assessment

Although guidance is provided for each specific endpoint separately, it should be remembered that different endpoints are related to each other. Information collected within one endpoint may influence hazard/risk assessment of other endpoints, e.g. information on a fast primary degradation of a parent compound may result in including the degradation products in the overall assessment of the toxicity of a substance. Similarly, information on toxicity/specific mode of action in one endpoint may indicate possible adverse effects for organisms considered for assessment of other endpoints, e.g. endocrine disrupting mode of action in mammals may indicate the same mode of action in fish. Another example may be when data on toxic effects measured in one group of organisms may be directly used in more than one endpoint, e.g. data from a repeated dose toxicity study may also be used in assessment of risk for secondary poisoning of mammals exposed via the food chains.

Adequacy of methods for generating additional information

Before proposing additional animal testing, use of alternative methods and all other options must be considered. It is important to emphasise that testing on vertebrate animals should

³ Council Regulation (EC) No 440/2008 laying down test methods pursuant to Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH)[OJ L 142, 31.5.2008, p. 1]

⁴ COUNCIL DIRECTIVE of 24 November 1986 on the approximation of laws, regulations and administrative provisions of the Member States regarding the protection of animals used for experimental and other scientific purposes (86/609/EEC)

⁵ Directive 2004/10/EC of the European Parliament and of the Council of 11 February 2004 on the harmonisation of laws, regulations and administrative provisions relating to the application of the principles of good laboratory practice and the verification of their applications for tests on chemical substances.

only be conducted or proposed as a last resort, when all other data sources have been exhausted (see, Recital 47 REACH, Article 25 REACH and Step 4, Annex VI to REACH). Therefore, it is important to first consider all issues that may impact upon this decision to perform the testing, such as:

- testing requirements,
- exposure/use pattern (emissions, yes or no, consumer use etc),
- occurrence (monitoring data),
- indications of the effect/ property based on animal or human data, *in vitro* data and non-testing information,
- any concern e.g. based on toxicokinetics, read-across and (Q)SAR considerations,
- WoE,
- seriousness of the effect,
- other effects of relevance for the endpoint.

All these issues should be considered, not only to design fit for purpose *in vivo* tests, but also for providing evidence for not performing *in vivo* testing under certain circumstances. Animal tests must comply with the provisions laid down in Council Directive 86/609/EEC⁶.

Degradation products and metabolites

In the context of evaluating substances for their effects, it is important to note that when they are released into the environment or taken up by animals, they may be transformed through degradation or metabolism. These processes and their outcome may need to be taken into account in the overall assessment.

Degradation products may be formed as a result of transformation processes in the environment. For distinguishing the substance undergoing degradation from the degradation products, the former is often referred to as the parent compound.

Degradation products may be formed as a result of abiotic environmental processes such as hydrolysis, direct or indirect photolysis or oxidation. They may also be formed as a result of aerobic or anaerobic biodegradation, i.e. due to microbial activity. Degradation products require further investigation if the Chemical Safety Assessment indicates the need, i.e. if stable degradation products are formed in the environment within a relevant time frame, as deduced from the test system, and in addition are so stable that they may result in risk, or if they are relevant considering in the PBT/ vPvB-assessment. Likewise it may be considered to assess whether degradation products fulfil the environmental hazard classification criteria (see Section R.7.9 in Chapter R.7(b): Endpoint specific guidance).

Metabolites refer to transformation products, which are formed due to biodegradation (and then the term metabolite is synonymous with the term biodegradation product) or formed as a result of biotransformation (metabolism) within exposed organisms after uptake of the parent

⁶ Council Directive 86/609/EEC regarding the protection of animals used for experimental and other scientific purposes [OJ L 358, 18.12.1986, p. 1]

1 compound. Metabolic pathways and hence the identity of many metabolites may or may not
2 be fully known. The latter is frequently the case. Moreover for the same substances metabolic
3 pathways may or may not differ between various organisms belonging to different phyla
4 and/or trophic levels. However, the toxicity of metabolites formed within the duration of
5 laboratory tests will with the exception of delayed effects showing up after the observation
6 time of the tests be reflected in such studies with their parent compound. Knowledge of
7 metabolic pathways and metabolites may increase planning and focussing of toxicity testing,
8 understanding of toxicological findings. (see Section R.7.12 in Chapter R.7(c): Endpoint
9 specific guidance) and may in some cases make it possible to use grouping approaches for
10 structurally closely related substances, which undergo similar metabolic transformation (see
11 Section R.6.2, Chapter R.6: Guidance on QSARs and grouping of substances).

12 Because many biotransformation processes includes oxidation, metabolites are often less
13 hydrophobic than the parent compound. This is a very general rule of thumb and may not
14 always apply; however, when it does, often this has implications for the hazard profile of the
15 metabolites. More polar metabolites created after oxidation processes have for example
16 normally a lower adsorption potential, and thus the relevance of the metabolites for the soil
17 and sediment compartments is normally lower than that of the parent compound. Such less
18 hydrophobic metabolites also tend to be excreted more rapidly from organisms than the parent
19 compound. Hence their bioaccumulative potential and narcotic toxicity tend to be less.

20 Similarities in metabolic pathways of structurally similar substances may serve as an alert or
21 waiving for further investigation depending of the case and nature of the metabolites.

22 Selection of the appropriate route of exposure for toxicity testing

23 Having comprehensively established the need for additional toxicity testing to meet the
24 requirements of REACH for a given substance, for certain endpoints, notably acute or
25 repeated dose toxicity but also reproductive toxicity, chronic toxicity and carcinogenicity, a
26 decision must be made on which route of exposure is most appropriate. The overall objective
27 of such testing is to establish the potential hazard of the test substance to human beings.
28 Humans may be exposed to substances by one or more of three routes: inhalation, dermal or
29 oral. Fundamentally, the use of the inhalation route of administration in animal tests should be
30 considered when inhalation exposure of humans is of relevance. However, the final decision
31 on which route of exposure to use in a particular test should be taken in the light of all
32 available information including physico-chemical properties of the substance, structure-
33 activity relationships (SAR) or the data from available toxicity tests on the substance itself.

34 Route-to-route extrapolation can be used to assess potential health effects and its threshold in
35 a route other than the one tested. Although toxicity data obtained using the appropriate route
36 of exposure are preferred. Route-to-route extrapolation should be considered on a case-by-
37 case basis and may introduce additional uncertainties, especially if the toxicity data were
38 obtained using an administration route that does not correspond to the most relevant route of
39 human exposure. In a subsequent risk assessment the uncertainties introduced through route-
40 to-route extrapolation should be taken into account, for example by adjusting the assessment
41 factor in the determination of the DNEL (see Section R.8.4.3, Chapter R.8: Characterisation
42 of dose [concentration]-response for human health). Further guidance on this strategic
43 approach to toxicity testing is given in Chapter R.8 Characterisation of dose [concentration]-
44 response for human health.

45 With regard to the evaluation of the environmental impact of a substance, the interaction of
46 that substance with the environment is an important consideration. The fate and behaviour of

a substance is largely governed by its inherent physicochemical properties. Knowledge regarding the physicochemical properties of the substance together with results from multimedia fate and transport models (e.g. Mackay level 3 models) enables the identification of the environmental compartment(s) of primary concern. Such information will also inform the prioritisation of higher tiered tests. More extensive guidance and considerations on this aspect are given in Chapter R.16: Environmental Exposure Estimation.

R.7.1 Physico-chemical properties

R.7.1.1 Introduction

According to Article 12 REACH, for substances registered all physicochemical information that is relevant and available to the registrant shall be included in the technical dossier, such as:

- Data for substance identification (e. g. melting point, vapour pressure, density, molecular size);
- Data to assess the physical hazards of a substance (e. g. flammability), with the view to determine its classification and labelling according to CLP (and according to DSD until June 1st 2015, see Article 61, CLP);
- Supplementary data for hazard assessment (e. g. viscosity, partition coefficient) and health and environmental classification.

Physicochemical properties can be subdivided into physical properties and physical hazards (see table R.7.1-1). For substances manufactured or imported in quantities of 100 tonnes or more, some additional physico-chemical data are required; in accordance with Annex IX to REACH (see also Table R.7.1-1).

In general, it is important that the data are as precise as possible. Several properties are inter-related; for example, water solubility and partition coefficient, vapour pressure and boiling point. The results of the respective tests can be used to check the validity of the data as specified in Annexes VII to IX to REACH.

Further details are given in section R.7.1.1.4 and in the sections dedicated to specific endpoints.

R.7.1.1.1 Information requirements on physico-chemical properties

Commission Regulation (EU) No 252/2011⁷ has amended Annex I to REACH in order to adapt the chemical safety assessment provisions to the criteria for classification laid down in the CLP Regulation. The relevant amendments have been applied since 5 May 2011; however, for registrations submitted prior to this date, the chemical safety report shall be updated in accordance with Regulation No 252/2011 by 30 November 2012 at the latest.

⁷ Commission Regulation (EU) No 252/2011 of 15 March 2011 amending Regulation (EC) No 1907/2006 of the European Parliament and of the Council on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) as regards Annex I

1 The information needed under Article 12, REACH and according to Annex VI, section 4 to
2 REACH, a physical hazard classification results from the application of the Title I and II CLP
3 and it is often complementary but in some cases may be different. The reason is that the
4 classification criteria and/or test methods under DSD and CLP regimes are different. This is
5 also expressed by the fact that CLP classifications are distributed over a different grid of
6 hazard classes and categories compared to the DSD regime, e.g. substances and mixtures
7 classified as explosive under DSD may be classified as explosives or self-reactives or organic
8 peroxides under CLP, or they may even be classified as flammable solids, oxidizing solids or
9 not at all. A translation table from DSD to CLP classification is provided in Annex VII, CLP
10 and an indication of potential classification outcomes under CLP compared to DSD
11 classifications is provided by Table 1.7.2.1(a) in the ‘*Guidance on the Application of the CLP*
12 *Criteria*’ which can be found on the following ECHA page:
13 [http://echa.europa.eu/web/guest/guidance-documents/guidance-on-the-different-methods-](http://echa.europa.eu/web/guest/guidance-documents/guidance-on-the-different-methods-under-reach)
14 [under-reach](http://echa.europa.eu/web/guest/guidance-documents/guidance-on-the-different-methods-under-reach).

15 The CLP classification regime is not explicitly considered in Annex VII to REACH and
16 therefore has to be understood as part of the information requirements under REACH. In
17 particular, certain headlines set out in column 1 of Annex VII, namely ‘explosive properties’,
18 ‘flammability’ and ‘oxidizing properties’, must be interpreted as covering the CLP hazard
19 classes that are referred to in CLP Article 58 (11).

20 As the physical hazards according to CLP are structured differently from the physico-
21 chemical properties according to DSD, some of the CLP hazard classes cannot be assigned to
22 only one of the information requirements according to REACH, Annexes VI to XI (for
23 example self-reactive substances have explosive and/or flammable properties). Therefore,
24 some of the hazard classes are listed twice in Table R.7.1-1 below. It should be noted that this
25 assignment is provided only as example and is done for the purposes of structuring this
26 guidance document according to CLP but nevertheless also allowing the assignment to the
27 respective information requirements according to Annexes VII to XI of REACH.

28 According to Art. 1 (6) CLP, CLP Regulation does not apply to the transport of dangerous
29 goods by air, sea, road, rail or inland waterways (save where the specific rules for labelling of
30 packaging applies under Art. 33 CLP). The transport of dangerous goods is, covered by the
31 UN Model Regulations for Transport of Dangerous Goods (UN-RTDG) and related legal
32 instruments (ADR, RID, ADN, IMDG Code and ICAO TI); the criteria listed in these
33 instruments and in CLP Regulation for classification purposes are intended to be the same.
34 Thus, a substance (or mixture) classified in a hazard class which is common to both CLP and
35 the transport legislation will normally be classified the same according to both systems.
36 However, the transport classifications do not include all of the GHS categories, so the absence
37 of a transport classification does not mean the substance (or mixture) should not be classified
38 under CLP. Therefore the transport classification of a substance could be a source of
39 information for the classification and labelling of substances (or mixture) under CLP for
40 physical hazards. Consequently in the case of a substance which has been tested for the
41 purposes of the UN-RTDG and for which the same procedure was followed as required by the
42 CLP Regulation, the same information could be used to comply with the REACH Regulation
43 on a case-by-case basis. The limitations to the approach described above are described in
44 detail in the ‘*Guidance on the Application of the CLP Criteria*’, Section 1.7.2.1.

45
46 For the preparation of the registration dossier, registrants are required to evaluate all the
47 information listed in Art. 10 REACH. Article 14 (1) in conjunction with Annex I and Article
48 10 (a)(vii) of the REACH Regulation, require the provision of a Robust Study Summary

(RSS) for information derived from the application of Annexes VI to XI To REACH In order to facilitate the evaluation conducted by the European Chemicals Agency and the Member States, as well as save resources of the registrant in case of a tonnage update, it is recommended that registrants also use the RSS for covering physico-chemical endpoints under section 4 of the IUCLID file. This guidance includes under each physico-chemical property or physical hazard chapter a list of detailed information to be given for each respective endpoint. Note that no further guidance is provided on the general aspects related to information common for all endpoints in IUCLID. For these further guidance is available in ‘*Practical guide 3: How to report robust study summaries*’ available on the ECHA Webpage: <http://echa.europa.eu/web/guest/support/documents-library> and in the IUCLID 5 End User Manual available on the IUCLID Webpage: <http://iuclid.eu/index.php?fuseaction=home.documentation#usermanual>.

Some endpoints (for example explosive, oxidising properties) are intimately linked to classification, which should be done according to CLP. For these endpoints, the test methods of CLP should preferably be used, in order to avoid double testing. For endpoints not linked to classification the preferred test methods are found in the Test Method Regulation. For some endpoints (for example flammability), more than one test procedure is referred to in the standard test method that is referred to in the Test Method Regulation. The one chosen should be suitable for the substance in question and be operating within its validity range. In the table below the preferred test method is highlighted in bold.

To distinguish between physical **properties** and physical **hazards**, the rows on physical hazards are gray shaded.

Table R.7.1-1 Information requirements as specified in Annexes VII to IX to REACH, CLP hazards classes and corresponding tests methods according to the Test Method Regulation and CLP

REACH Regulation (EC) No. 1907/2006 (the no. in brackets is the respective no. in the table in Annex VII to XI to REACH)	Corresponding test method according to the Test Method Regulation 440/2008	Chapter in revised R.7(a) guidance	CLP Regulation (EC) No. 1272/2008 (the no. in brackets is the respective chapter no. in Annex I to CLP)	Corresponding test method according to the CLP Regulation
Melting/Freezing point (7.2)	A.1 Melting/Freezing temperature	7.1.2	/	/
Boiling point (7.3)	A.2 Boiling temperature	7.1.3	/	CLP Annex I chapter 2.6.4.6
Relative density (7.4)	A.3 Relative density	7.1.4	/	/
Vapour pressure (7.5)	A.4 Vapour pressure	7.1.5	/	/
Surface tension (7.6)	A.5 Surface tension	7.1.6	/	/
Water solubility (7.7)	A.6 Water solubility	7.1.7	/	/
Partition coefficient n-octanol/water (7.8)	A.8 Partition coefficient	7.1.8	/	/
Flash point (7.9)	A.9 Flash-Point	7.1.9	/	CLP Annex I chapter 2.6.4.4
Flammability (7.10)	A.11 Flammability (gases)	7.1.10.1	Flammable gases (2.2)	ISO 10156 EN 1839
	/	7.1.10.2	Flammable aerosols (2.3)	UN Section 31
	for flammable	7.1.10.3	Flammable	see Flash point and

	liquids: see Flash point and Boiling point		liquids (2.6)	Boiling point
	A.10 Flammability (solids)	7.1.10.4	Flammable solids (2.7)	UN Test N.1
	/	7.1.10.5	Self-reactive substances and mixtures (2.8)	UN Test series A to H
	A.13 Pyrophoric properties of solids and liquids	7.1.10.6	Pyrophoric liquids (2.9)	UN Test N.3
		7.1.10.7	Pyrophoric solids (2.10)	UN Test N.2
	/	7.1.10.8	Self-heating substances and mixtures (2.11)	UN Test N.4
	A.12 Flammability (Contact with water)	7.1.10.9	Substances and mixtures which in contact with water emit flammable gases (2.12)	UN Test N.5
	/	7.1.10.10	Organic peroxides (2.15)	UN Test series A to H
Explosive properties (7.11)	A.14 Explosive properties	7.1.11.1	Explosives (2.1)	UN Test series 1 to 3 (further test series 4 to 6 are necessary for classification)
	/	7.1.11.2	Self-reactive substances and mixtures (2.8)	UN Test series A to H
	/	7.1.11.3	Organic peroxides (2.15)	UN Test series A to H
Self ignition temperature (7.12)	A.15 Auto-ignition temperature (liquids and gases)	7.1.12.1	For gases and liquids	/
	A.16 Relative self-ignition temperature for solids	7.1.12.2, 7.1.10.8	For solids	/
Oxidising properties (7.13)	/	7.1.13.1	Oxidising gases (2.4)	ISO 10156
	A.21 Oxidising properties (liquids)	7.1.13.2	Oxidising liquids (2.13)	UN O.2
	A.17 Oxidising properties (solids)	7.1.13.3	Oxidising solids (2.14)	UN O.1
Granulometry (7.14)		7.1.14	/	
Adsorption/Desorption (7.15)		7.1.15	/	
Stability in organic solvent and degradation products (7.16)		7.1.16	/	
Dissociation constant (7.17)		7.1.17	/	
Viscosity (7.18)		7.1.18	/	
Not listed in Annex VII to REACH		7.1.19.1 (Parameters only appearing in the CLP	Gases under pressure (2.5)	

		Regulation)		
		7.1.19.2 (Parameters only appearing in the CLP Regulation)	Corrosive to metals (2.16)	UN Test C.1 (section 37.4)

The REACH information requirements have to take due account of the waiving according to column 2 of the tables in Annexes VII to XI to REACH, which has to be understood and applied in relation to the appropriate CLP hazard class. Further adaptations according to Annex XI to REACH must then be read together with the waiving possibilities provided by Article 8 (2) CLP and the CLP criteria themselves, namely Annex I, Part 2 of CLP.

Physico-chemical data are mostly numeric and should be provided in SI units. Normally a numeric value or range is required. Where relevant, additional information should be provided, such as the relevant testing conditions (temperature and/or pressure and/or concentration etc.). Furthermore details of any observations made during testing should be reported, e.g. decomposition during melting or boiling, emulsion formation during partitioning.

R.7.1.1.2 Available information on physico-chemical properties

There are many published sources of data for basic substance characterisation and of supplementary information for hazard assessment. The relevant references are listed under respective endpoint.

R.7.1.1.3 Evaluation of available information on physico-chemical properties

Experimental data

Pursuant to Article 13 (3) REACH, testing should be carried out according to the test methods laid down in a Commission Regulation or in accordance with other international test methods recognised by the Commission or the Agency as being appropriate. The test methods for the physico-chemical properties are described in Regulation (EC) No 440/2008, whereas tests for the purposes of physical hazard classification are referred to in the CLP Regulation Annex I, Part 2 (via references to the UN Manual of Tests and Criteria and to applicable standards). In Table R.7.1-1 the preferred test method is highlighted in bold. The test methods referred to in the CLP Regulation are also used for the transport of dangerous goods. Therefore, available information on physico-chemical properties and physical hazards may also originate from tests that were carried out for the purposes of classification for transport. Such test data may be used for the information requirements according to REACH. It should, however, be kept in mind that the classification for transport does not cover all hazard categories which are relevant for CLP and it may be based on other considerations than just the test data and criteria (e.g. classifications which are based on experience rather than testing or which apply only in connection with certain special provisions). As a result transport classifications may be different from the classification according to CLP. Such limitations are described in detail in the '*Guidance on the Application of the CLP Criteria*', Section 1.7.2.1.

Where relevant recognised standards for testing are applicable, the use of the most recent updates is advised; they are accessible via numerous websites, for example:

1. EN standards;

2. [ISO standards](#);

3. [IEC standards](#).

The national editions of the EN or ISO standards are available via the national standardization organizations accessible via the [CEN Website](#).

Non-experimental data

Quantitative Structure Property Relationships (QSPR) models exist for some of the physico-chemical endpoints. Where applicable the details of any specific QSPR models are given under each endpoint.

The majority of QSPR models have been built using training sets of substances. The model will have been optimised to calculate values for the training substances that most closely match measured ones. Therefore, the use of QSPR estimation techniques requires expert judgment. The calculated values need to be checked to ensure that they are reasonable and that the model used is appropriate.

A valid model will give values that are in reasonably close agreement with the measured ones for your chosen analogue substances (i.e. the substance with a data gap should have similar substances in the training set of the model). The models may not predict well chemistry, which they don't know. Thus, the model can be used to provide a predicted value for your substance without the need for testing. Another check is that the values are reasonable. This can be done by cross-referencing the calculated value to measured values for similar substances and related endpoints.

Uncertainty evaluation of data

Test data have an uncertainty of measurement. Some test methods include information about their uncertainty, which then may be referred to for test data generated using these test methods. Where the uncertainty of measurement is not specified by the test method, the uncertainty should be determined (e.g. according to ISO/IEC Guide 98-3:2008).

Quality assurance for the determination of physico-chemical properties

Test data on physical-chemical properties should be of sufficient quality i.e. they must be adequate and reliable. Normally this can only be achieved by testing that is carried out in compliance with a relevant recognised quality system (e.g. GLP) or by laboratories complying with a relevant recognised standard (e.g. EN ISO/IEC 17025). Under Art. 8(5) CLP, where new tests for physical hazards are required for the purposes of CLP they have to be carried out in compliance with a relevant recognised quality system or by laboratories complying with a relevant recognised standard at the latest from January 1st, 2014.

Use of secondary and historical data sources for physico-chemical properties

The reliability of data must be demonstrated by providing information on the identity and purity of the test substance, the methodology used to make the measurement, and whether or not this was performed to GLP standards (Annex VI, REACH).

1 Assessing the quality of QSPR models

2 The European Commission and the OECD member countries adopted five principles for the
3 validation of (Q)SAR/(Q)SPR models in 2004 (OECD^a, 2004). According to these principles,
4 a valid (Q)SPR model should have 1) a defined endpoint whose experimental conditions are
5 clearly specified; 2) an unambiguous algorithm; 3) a defined domain of applicability that
6 defines for what kind of substances predictions can be made; 4) appropriate measures of
7 goodness-of-fit, robustness and predictivity; and 5) a mechanistic interpretation if possible.
8 These principles are outlined on the ECB website and more extensively covered in IR/CSA
9 R.6: QSAR and grouping of substances, section R.6.1.3. Moreover, a practical overview of
10 these principles is given in the report from the expert group on (Q)SARs (OECD^c, 2004).

11 Assessing the quality of read-across predictions

12 This paragraph reports the basic concepts of a read-across approach. Thorough information on
13 this topic can be found in the guidance on the grouping of substances (see IR/CSA R.6:
14 QSAR and grouping of chemicals, Section R.6.2).

15 A read-across/analogue approach assesses the relevance of a given property on one or more
16 chemical structures and then makes some assessment (qualitative or quantitative) on the
17 relevance of this information for another substance (see Annex XI, REACH). Since a read-
18 across may involve two substances^s it is of paramount importance to detail the reasoning
19 behind the inference on the substance whose property is unknown. An analogue must:

- 20 • contain the same major structural features and the same functional groups as the
21 substance under investigation;
- 22 • have a physico-chemical profile comparable to that of the substance under
23 examination as far as the known physico-chemical properties are concerned;
- 24 • have comparable values for the relevant molecular descriptors (i.e. excess molar
25 refractivity and hydrogen bond donor and acceptor abilities for water solubility
26 predictions) generally used for the quantification of the property of interest;
- 27 • have approximately the same molecular weight.

28 The interpretative analysis of a read-across is usually the result of an expert judgement
29 evaluation and detailed documentation should therefore always be provided to support the
30 conclusions. It is important to point out that, in practice, read-across for physico-chemical
31 properties is not generally recommended, since reliable data should normally be available or
32 easily obtainable (Article 8 (2), CLP).

33 Measured values which are evaluated in reviews and assigned recommended values are given
34 precedence over calculated values. The major criteria that characterise the analysis of the
35 available information are:

- 36 a) *Experimental data*. When assessing physico-chemical properties, priority is given to first
37 hand experimental results or to primary references provided that the methods are suitable

^s A read-across can also involve more than two chemicals: one-to-one (one analogue used to make an estimation for a single chemical) b) many-to-one (two or more analogues used to make an estimation for a single chemical) c) one-to-many (one analogue used to make estimations for two or more chemicals) d) many-to-many (two or more analogues used to make estimations for two or more chemicals)

for the substance under investigation and that they operate within their validity range. Proper documentation on the methods and the inherent uncertainty of the measurements should also be provided.

- b) *Non-testing information*. If the information described in point (a) is not available, QSPRs, read-across or secondary data sources can be used in accordance with the limitations described in the individual endpoint chapters (7.2 to 7.19 in this guidance) instead.

R.7.1.1.4 General testing strategy for physico-chemical properties/hazards

When testing is to be carried out there are advantages in considering the order in which testing should be done. For example:

- Some tests can be omitted when the results from another tests are available.
- There are safety implications to consider when performing tests on substances that have certain hazardous properties.
- In some tests, better quality results can be obtained through prior knowledge of related properties.

The following flow-charts intend to outline a testing strategy which considers these advantages and which can be used depending on the type of substance under investigation and the properties/hazards on which reliable information is already available. In some cases it might be appropriate to follow a different approach or there may be some (rare) exceptions that are not covered correctly by the flow-chart. The flow-chart should be understood only as a guidance for the testing strategy, and especially the order in which testing is carried out. It cannot be understood as a decision logic with regard to classification and precedence of hazards. Detailed information on each physical-chemical property/hazard can be found in the following chapters R.7.1.2 to R.7.1.19.

The flow-charts should be read as follows:

- In the flow-charts each bullet point stands for a physical-chemical property which is explicitly named in Annex VII or Annex IX to REACH. Each of these properties and the respective information requirements and waiving possibilities are described in a specific chapter of this document.
- Information on properties without a bullet point (this concerns the critical temperature in Flow-chart 1) is not explicitly required by REACH. However, it is recommended to include this information as well.
- The order of testing for bullet points which are in one and the same box is not important and can be adjusted. However, the order given is a recommendation.
- Testing is not necessarily required for every bullet point that is passed via the flow-chart because waiving might be possible (e.g. a ‘normal’ flammable liquid would not be tested for explosive properties based on the oxygen balance). Information on waiving is given in the individual chapters for the respective property/hazard.

FLOW-CHART 1 – TESTING STRATEGY FOR GASES

The following additional explanations are important in connection with flow-chart 1:

- Gases are substances that have a vapour pressure of more than 300 kPa (absolute) at 50 °C or that are completely gaseous at 20 °C and a standard pressure of 101,3 kPa.
 - Critical temperature
- Although not explicitly required by REACH, it is recommended to include information on the critical temperature of gases because this information is needed for the assignment of the group (category) for gases under pressure according to CLP.

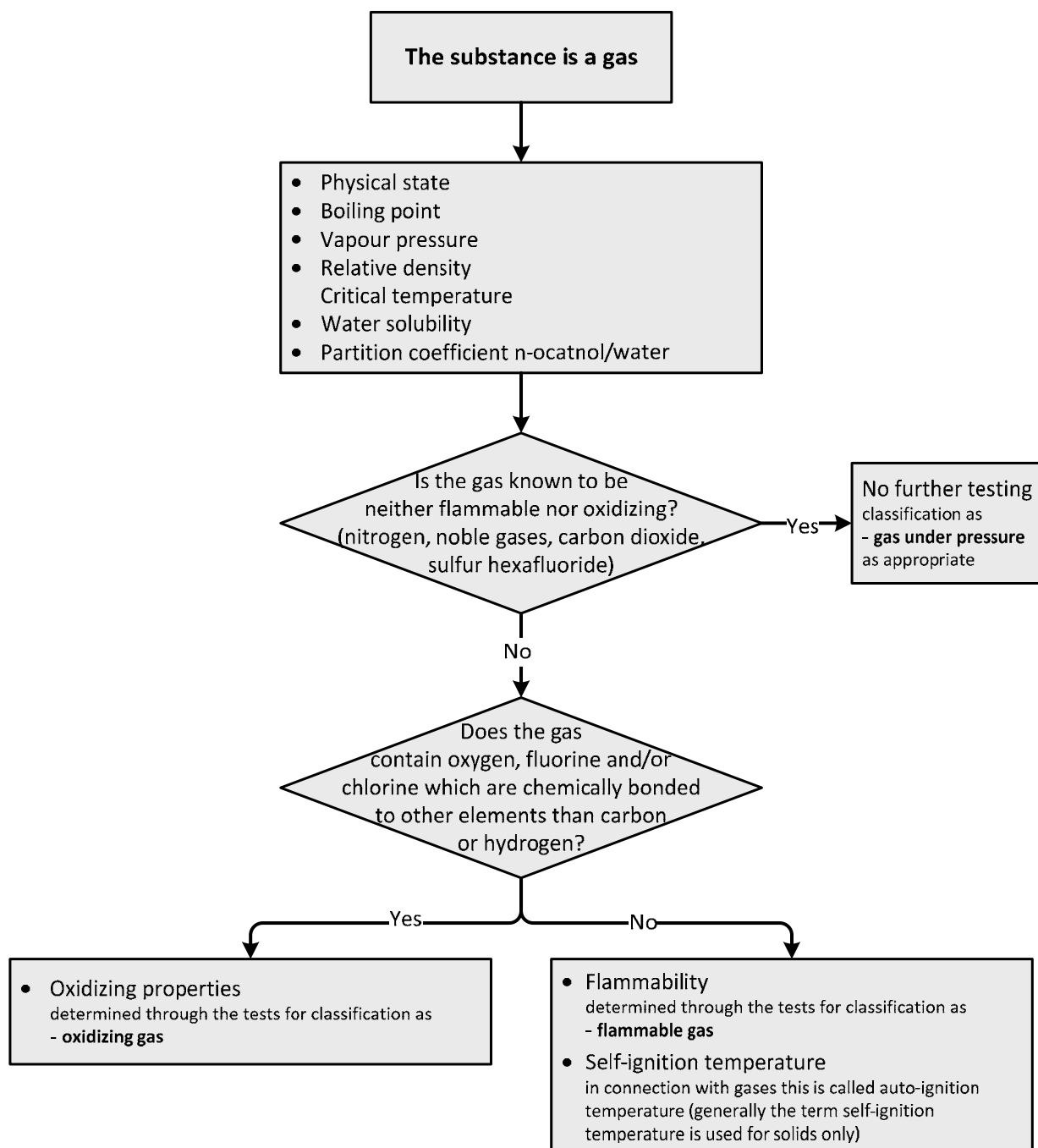


Figure xxx :Flow-chart 1 Testing strategy for gases

FLOW-CHART 2 – TESTING STRATEGY FOR LIQUIDS AND SOLIDS

The following additional explanations are important in connection with flow-chart 2:

- Liquids are substances that are not gases (see above) and that have a melting point or initial melting point of 20 °C or less at a standard pressure of 101.3 kPa.
- Solids are substances that are neither gases nor liquids.
- Pyrophoric substances
Normally, not all properties are determined for pyrophoric substances, however, some may be well determined under inert gas and some methods explicitly require testing under inert gas for pyrophoric substances (e.g. classification of a pyrophoric substance as water-reactive according to UN Test N.5).
- Explosive properties
Information requirements on explosive properties are linked to several CLP hazard classes (explosives, self-reactive substances and mixtures, organic peroxides, but in some cases also flammable solids, oxidizing solids or corrosive to metals may have explosive properties). In addition, it is important to identify possible explosive properties with regard to safety in further handling and testing of a substance at the very beginning of the testing program of a substance. This is the purpose of the box in the top right corner of Flow-chart 2 which shall ensure that explosive properties are determined before other tests, especially with larger amounts, are carried out. Explosive properties are mainly determined by test series 2 according to the UN Manual of Tests and Criteria, however, this does not cover the mechanical sensitivity which is also important in the course of further handling/testing of the substance. Therefore, it is recommended to test for the mechanical sensitivity first. Testing for the mechanical sensitivity (sensitiveness to impact and to friction) can be done by using test series 3 with adapted criteria (for details and criteria see chapter R.7.1.11). Information requirements with regard to explosive properties are covered at later stages in the flow-chart but of course the information as gained at the start will also be useful later (see chapter R.7.1.11).
- Intentional explosives
Intentional explosives are substances mixtures or articles which are manufactured with a view to producing a practical, explosive or pyrotechnic effect (CLP Annex I, section 2.1.1.2).
- Screening for explosive properties
Screening procedures for explosive properties are described in the UN Manual of Tests and Criteria, Appendix 6.
- Flammability
Flammability is mainly determined through the various tests for the classification of substances. However, in some cases a substance might have flammable properties without that it is classified accordingly, e.g. some halogenated hydrocarbons such as methylene chloride.
- Thermally unstable substances
Substances are considered as thermally unstable if their heat of decomposition is ≤ 300 J/g and their self-accelerating decomposition temperature (SADT) is ≥ 75 °C for a 50 kg

1 package (meaning they are to be considered for classification as a self-reactive
2 substance or mixture).

- 3 • Self-ignition temperature
4 Annex VII to REACH explicitly names the self-ignition temperature (column 1, section
5 7.12). However, in connection with gases and liquids this is called auto-ignition
6 temperature.

7

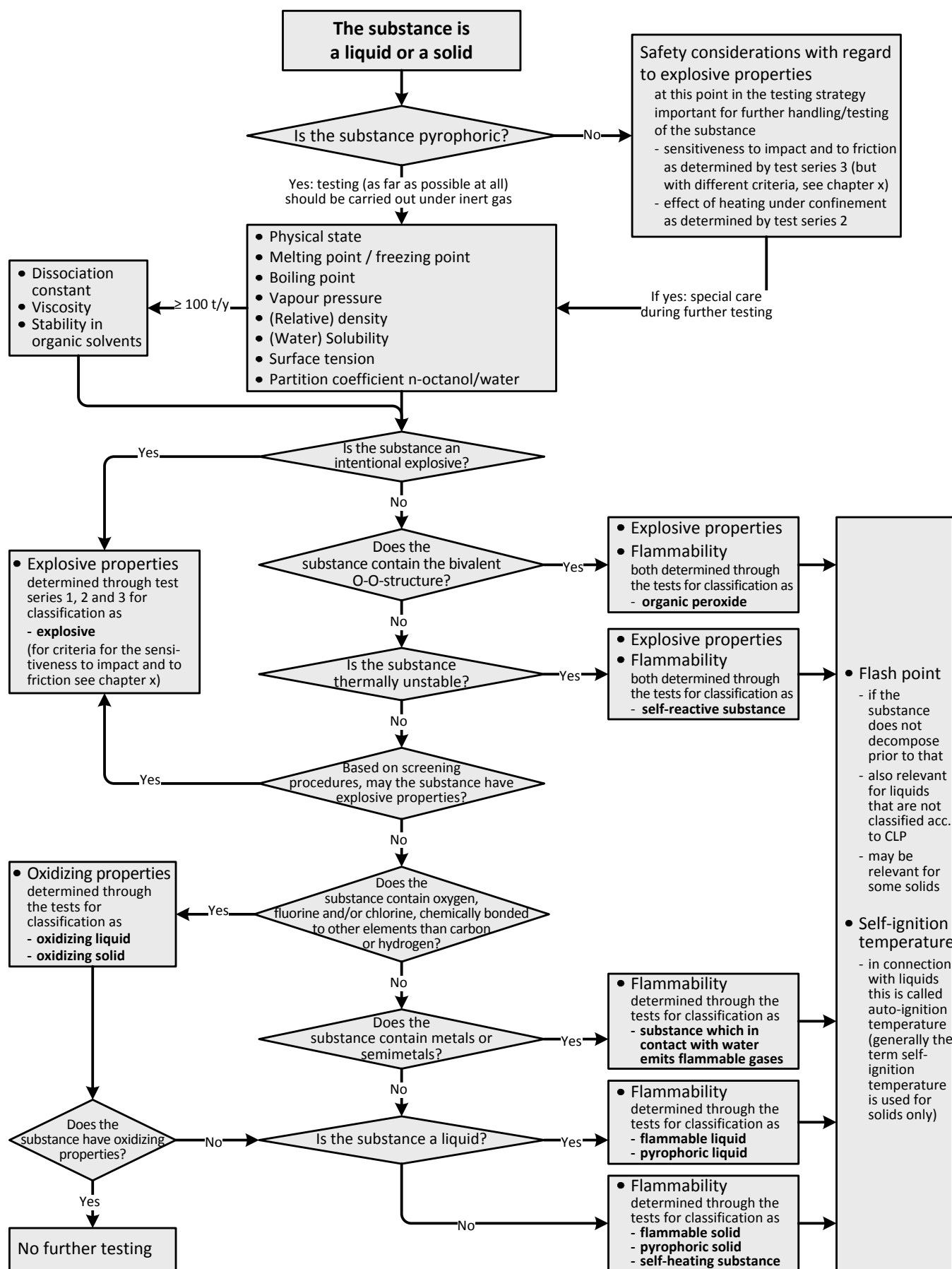


Figure xx: Flow-chart 2 Testing strategy for liquids and solids

R.7.1.1.5 Overall consistency of the physico-chemical profile

The physico-chemical profile for a given substance cannot contain incompatible values for two or more properties (i.e. high boiling point and high vapour pressure at normal temperature) This consistency check should be always done and it can turn out to be particularly useful when measured values are significantly at odds with predictions from QSPR models. Indeed, in this case a wider assessment of the known physico-chemical properties should be performed in order to determine the possible cause of the inconsistencies.

Concluding on classification and labelling and chemical safety assessment

Physico-chemical data are also necessary for the environmental and human health sections of the chemical safety assessment. The assessment determines the risk posed to humans and the environment from all stages of the substance's lifecycle. This includes its manufacture, transport, use and disposal. For example, the vapour pressure and the particle size determination are required to estimate the likely exposure of humans both in the workplace and in consumer use. Exposure estimates the volatility (vapour pressure) or the size and nature of particles to estimate inhalation exposure. Particle size is also important for determining the likely dermal exposure. Viscosity is a key parameter in determining aspiration hazards. The physical state of a substance at the process temperature is important for determining possible hazards.

Table R.7.1-2 Summary of use of physico-chemical properties

Test	Impact on other Physico-chemical tests	Impact on toxicology	Impact on Ecotoxicology	Impact on Risk assessment
Melting/freezing point	<p>Relevant for decision about the physical state. As such also relevant with regard to physical hazard classification.</p> <p>Relevant for the applicability of test methods such as</p> <ul style="list-style-type: none"> - flash point - auto-ignition / self-ignition temperature - oxidising properties - explosive properties (sensitivity to friction). <p>If decomposition occurs during testing of the melting point, the boiling point need not be measured.</p>			Indicates (together with the boiling point) the physical state of a compound.
Boiling point	Relevant for decision about the physical state. As such also relevant			Indicates (together with the melting/freezing point) the physical

Test	Impact on other Physico-chemical tests	Impact on toxicology	Impact on Ecotoxicology	Impact on Risk assessment
	with regard to physical hazard classification. In addition affects classification as flammable liquid cat 1 or cat 2. Related to the vapour pressure			state of a compound. Need to consider process temperature for risk assessment.
Relative density			To decide if an immiscible compound floats in water or sinks to the bottom.	Fire-fighting measures: H ₂ O extinguishers may not be suitable if $D_{4}^{20} < 1$
Vapour pressure	Extra care needed to minimise vapour losses. Related to boiling point.	Choice of dermal or inhalation exposure route for acute toxicity test. Route of exposure for sub-acute toxicity test. Exposure and excretion routes for toxicokinetic assessment. It enables a statement about inhalative absorption in the living organism.	Choice of test method for biodegradation test. Closed/covered vessels for ecotoxicity tests	Health risk assessment. Calculation of Predicted Environmental Concentrations (PECs) for environmental risk assessment- vapour pressure is a key parameter in determining environmental fate and behaviour. Determination of atmospheric behaviour as for exposure of man via the environment calculations.
Surface tension	Suitability of methods for K_{ow} and K_{oc} determination for surface-active substances. Can occasionally interfere with measurement of	Cellular disruption. Surface active substances have a higher local irritant or corrosive effect. As a consequence of local corrosion		Environmental fate.

Test	Impact on other Physico-chemical tests	Impact on toxicology	Impact on Ecotoxicology	Impact on Risk assessment
	water solubility.	the dermal uptake of a substance can be enhanced		
Water solubility	Surface tension test not applicable for $WS < 1 \text{ mg/l}$. Need to prepare 90 % saturated solution (up to a maximum of 1 g/l) for surface tension test. Time to achieve saturation can be relevant to solution preparation for surface tension test. Water solubility affects concentration used in hydrolysis test	Toxicokinetic behaviour.	Sample preparation for ecotoxicity tests.	Environmental classification and labelling. PEC calculations – water solubility is a key parameter in determining environmental fate and behaviour.
Partition coefficient n-octanol/water	Generally, substances with a high $\log K_{ow}$ will be hydrophobic and have low water solubilities. Substances with negative $\log K_{ow}$ will be hydrophilic and have high water solubilities.	Toxicokinetic behaviour: It indicates the potential for absorption across biological membranes and for passive diffusion. It provides information on the potential for accumulation in the body. Suitable vehicle for toxicity studies. Prediction of dermal absorption.	Choice of test method for biodegradation test (some are not suitable for substances which have high adsorption) High $\log K_{ow}$ may lead to losses in ecotoxicity tests through adsorption. Bioaccumulation and adsorption potential. Toxicity prediction.	Environmental classification and labelling. PEC calculations – $\log K_{ow}$ is a key parameter in determining environmental fate and behaviour and is used as a surrogate for bioaccumulation potential in the absence of bioaccumulation tests.
Granulometry		Computation of inhalable, thoracic and respirable fractions as a function of size of		

Test	Impact on other Physico-chemical tests	Impact on toxicology	Impact on Ecotoxicology	Impact on Risk assessment
		particles.		
Adsorption/desorption			As for log K_{ow}	log K_{oc} is a key parameter in determining environmental fate and behaviour.
Dissociation constant	Interpretation of results for surface tension, K_{ow} and K_{oc} tests and water solubility.	Exposure to hydrolysis products <i>in vivo</i> . It indicates the potential for absorption from the gastrointestinal tract, because ionised compounds are thought not to cross biological membranes.	Preparation of test solutions for ecotoxicity tests. Interpretation of ecotoxicity results.	Influences PEC calculation.
Viscosity	Choice of methods for the determination of density.	Parameter for aspiration hazard		Assessment of spreadability of liquids

1 R.7.1.1.6 References for introduction of Physico-Chemical properties

- 2 Dearden J.C. *In silico* prediction of aqueous solubility. *Expert Opinion on Drug Discovery* 1 (2006)
3 31-52.
- 4 Eriksson, L., Jaworska, J., Worth, A.P., Cronin, M.T.D., McDowell, R.M., Gramatica, P.(2003).
5 Methods for reliability and uncertainty assessment and for applicability evaluations of classification
6 and regression-based QSARs. *Environ. Health Perspect.* 111, 1361-1375.
- 7 Gerstl Z. Estimation of organic chemical sorption by soils. *J. Contaminant Hydrology* (1990) 6,
8 357-375 .
- 9 Katritzky AR, Wang Y, Sild S and Tamm T. QSPR studies on vapour pressure, aqueous solubility,
10 and the prediction of water-air partition coefficients. *J. Chem. Inf. Comput. Sci.* 38 (1998) 720-725.
- 11 OECD^a (2004) Principles for the Validation of (Q)SARs
12 [http://ecb.jrc.it/QSAR/home.php?CONTENU=/QSAR/background/background_oecd_principles.ph](http://ecb.jrc.it/QSAR/home.php?CONTENU=/QSAR/background/background_oecd_principles.php)
13 [p](http://ecb.jrc.it/QSAR/home.php?CONTENU=/QSAR/background/background_oecd_principles.php)
- 14 OECD^c (2004) series on testing and assessment Number 49 The report from the expert group on
15 (quantitative) structure activity relationships [(Q)SARs] on the principles for the validation of

(Q)SARs. 2nd Meeting of the ad hoc Expert Group on QSARs
[http://applied.oecd.org/olis/2004doc.nsf/linkto/env-jm-mono\(2004\)24](http://applied.oecd.org/olis/2004doc.nsf/linkto/env-jm-mono(2004)24)

Tetko, I.V., Bruneau, P., Mewes, H.W., Roher, D.C., Poda, G.I. (2006). Can we estimate the accuracy of ADME-Tox predictions? *Drug Disc. Today* 15/16, 700-707

Vracko, M., Bandelj, V., Barbieri, P., Benfenati, E., Chaudhry, Q., Cronin, M., Devillers, J., Gallegos, A., Gini, G., Gramatica, P., Helma, C., Mazzatorta, P., Neagu, D., Netzeva, T., Pavan, M., Patlewicz, G., Randic, M., Tsakovska, and Worth, A. (2006). Validation of counter propagation neural network models for predictive toxicology according to the OECD principles: a case study. *SAR and QSAR in Environ. Res.* 3, 265-284.

Walker J.D., Jaworska J., Comber M.H.I., Schultz T.W. and Dearden J.C. Guidelines for developing and using quantitative structure-activity relationships. *Environ. Toxicol. Chem.* 22 (2003) 1653-1665.

R.7.1.2 MELTING/FREEZING POINT

R.7.1.2.1 Type of property

The melting point serves as an indicator for the physical state (liquid or solid) of a substance. A number of physical hazard classes are distinguished based on the physical state. Therefore the melting point of a substance and the consequent designation as liquid or solid also has consequences for the assignment of the correct hazard class. With regard to environmental relevance the melting point can give an indication of the distribution of the substance within and between the environmental media water, soil and air.

R.7.1.2.2 Definition

The melting temperature is defined as the temperature at which the phase transition from the solid to the liquid state occurs at atmospheric pressure and this temperature ideally corresponds to the freezing temperature. As the phase transition of many substances takes place over a temperature range, it is often described as the melting range.

R.7.1.2.3 Test method(s)

Method A.1 of Regulation EC 440/2008 or OECD Test Guideline 102 should be generally used for testing. Any procedure given in A.1 may be used within the scope and applicability specifications. However, it is advisable to use the Differential Scanning Calorimetry (DSC) or DTA method since they give additional information about the thermal stability of the substance like decomposition onset and energy. If decomposition occurs during the melting point study, determination of the boiling point need not be carried out.

R.7.1.2.4 Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

Annex VII to REACH does not require determination of the melting point below a lower limit of -20 ° C. The lower limit should be confirmed through testing, except where a (Q)SAR indicates a melting point of -50 ° C.

Waiving possibilities according to Annex XI to REACH

Use of existing data: Data on physical-chemical properties from experiments not carried out according to GLP or the test methods referred to in Article 13 (3) of REACH

The melting point does not have to be determined experimentally if conclusive and consistent literature data are available.

Weight of evidence

For the determination of the melting point, weight of evidence is not possible.

(Q)SAR

For the determination of the melting point, (Q)SAR approaches are discouraged, because the accuracy is not sufficient ($\pm 25\text{ }^{\circ}\text{C}$ to $30\text{ }^{\circ}\text{C}$) for the purposes of classification / risk assessment.

Grouping of substances and read-across approach

For the determination of the melting point read across is not possible.

Testing is technically not possible

Some substances will decompose or sublime before the melting point is reached. For some substances, the determination of the freezing or solidification point is more appropriate. Where due to the particular properties of the substance, none of the above parameters can be conveniently measured, a pour point may be appropriate.

Further waiving possibilities

Not foreseen.

R.7.1.2.5 Impurities; uncertainties

Impurities can have a significant influence on the melting point, as they will generally lower the melting point noticeably. Therefore utmost care should be taken in the use of literature data as literature and handbook data are generally relevant for pure substances only (unless stated otherwise).

R.7.1.2.6 Endpoint specific information in the registration dossier/ IUCLID

Materials and methods

- type of method or reference to the standard or the test method applied.

Results and discussion

- melting point value ($^{\circ}\text{C}$) as measured;
- rate of temperature increase;
- decomposition or sublimation temperature (if applicable);
- uncertainty in measurement.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on melting point/freezing point can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.2	VII 7.2	Melting point/freezing point	E.4.3	3.2

R.7.1.3 BOILING POINT

R.7.1.3.1 Type of property

The boiling point is a property:

- for substance characterization including physical state (gas or liquid);
- which is the basis for the assignment of the correct hazard class because a number of physical hazard classes are distinguished based on the physical state;
- which is needed for the classification of flammable liquids into categories;
- which gives an indication of the distribution of the substance within and between air and water or soil.

R.7.1.3.2 Definition

The normal boiling point is the temperature at which the vapour pressure of a liquid equals 101.3 kPa.

Note: If the vapour pressure equals 101.3 kPa this means the substance is completely gaseous at that temperature. If this is the case at temperatures ≤ 20 °C the substance is a gas also according to the CLP Regulation.

R.7.1.3.3 Test method(s)

Method A.2 of Regulation EC 440/2008 or OECD Test Guideline 103 should be used for testing. Any determination method may be used within the scope and applicability specifications. DSC can be used to evaluate the melting and boiling point in a single test. For some substances a single test can provide both endpoints ‘boiling point’ and ‘vapour pressure’ because they are closely related.

For high-boiling liquids or liquids which may decompose, auto-oxidize etc. before the boiling point at 101.3 kPa is reached, it is recommended to determine the boiling point either under inert gas or at reduced pressures respectively to derive the boiling point at reduced pressures from the vapour pressure curve.

If explosives, pyrophorics or self-reactives are to be characterized, determination of the boiling point is in general not practicable. For pyrophorics testing under inert gas or reduced pressures should be considered.

Where standards are applicable, the use of the most recent updates is advised; they are accessible via numerous websites, see above in section R.7.1.1.3.

R.7.1.3.4 Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

Column 2 of REACH Annex VII provides the following specific rules for adaptation of the standard information requirement for boiling point:

The study does not need to be conducted if:

– for gases; or

– for solids which either melt above 300°C or decompose before boiling. In such cases the boiling point under reduced pressure may be estimated or measured; or

– for substances which decompose before boiling (e.g. auto-oxidation, rearrangement, degradation, decomposition, etc.).

Therefore the Annex VII to REACH does not require determination of the boiling point if:

- The substance is a gas;

However, for some gases the boiling point may be relevant. In the CLP Regulation, the boiling point is the main criterion to distinguish gases from liquids (see Annex I, 1.0 ‘Gas means a substance which(i) at 50 °C has a vapour pressure greater than 300 kPa (absolute); or (ii) is completely gaseous at 20 °C at a standard pressure of 101.3 kPa’). Therefore it is important to report the boiling point in borderline cases where the transition from liquid to gas occurs close to 20°C.

- The melting point of the substance is above 300 °C or when it decomposes before boiling;

- The substance decomposes before boiling at ambient pressure;

In such cases the boiling point under reduced pressure (down to 0.2 kPa) should be determined if possible without decomposition.

Waiving possibilities according to Annex XI to REACH

Use of existing data: Data on physical-chemical properties from experiments not carried out according to GLP or the test methods referred to in Article 13 (3) of REACH

The use of existing experimental data is possible if carried out by certified institutions.

Weight of evidence

For the determination of the boiling point, weight of evidence is not possible.

(Q)SAR

For the determination of the boiling point, (Q)SAR approaches are discouraged for the purpose of classification / risk assessment, except when the mean absolute error of the method is lower than 2 K.

Grouping of substances and read-across approach

For the determination of the boiling point read across is not possible. Interpolation within homologous series may however be possible.

Testing is technically not possible

Testing is not possible if:

- the substance is an explosive;
- the substance is self-reactive;
- decomposition occurs during the melting point study;
- the liquid decomposes before the boiling point is reached even at reduced pressures below 0,2 kPa.

In such cases the decomposition temperature in relation to the (reduced) pressure and the details of the determination method should be reported.

Further waiving possibilities

The boiling point does not have to be determined experimentally if conclusive and consistent literature data are available. Data generated with the same tests and classification principles as specified in the CLP Regulation on viscosity generated in conjunction with transport classification can be deemed to satisfy the REACH requirements on a case-by-case basis.

R.7.1.3.5 Impurities; uncertainties

Impurities can have a significant influence on the boiling point. The influence depends on the amount and boiling point of the impurity. The higher the amount and the higher the difference between the boiling points of the main component and the impurity, the higher the influence. This has to be kept in mind and taken into account when taking data from literature as those are generally relevant for pure substances only, unless stated otherwise.

R.7.1.3.6 Endpoint specific information in the registration dossier / in IUCLID

Materials and methods

- type of method or reference to the standard or the test method applied.

Results and discussion

- boiling point value (°C) as measured;
- pressure value and unit;
- rate of temperature increase;
- decomposition (if applicable);
- uncertainty in measurements ;
- boiling point value in °C (corrected to standard pressure, except where the boiling point has been determined at specified reduced pressures) (as above, but in a separate block of fields).

Note: In case the boiling point is determined at reduced pressure a determination at ambient pressure is not possible. A boiling point at standard pressure could then only be derived by extrapolation of the vapour pressure curve in cases where a vapour pressure curve is known. Even in such cases this corrected/extrapolated boiling point could only be nominal one and would be potentially misleading because it is not possible to determine it at ambient pressure.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on boiling point can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.3	VII 7.3	Boiling point	E.4.4	3.2

R.7.1.4 RELATIVE DENSITY

R.7.1.4.1 Type of property

For gaseous materials, density is of value in determining the tendency to settle or to disperse when discharged at high concentrations into the atmosphere. The density of gaseous substances can be calculated from molecular weight using the gas law.

For insoluble liquids and solids, density will be a determining factor in the settling of the substance.

R.7.1.4.2 Definition

Density (ρ) of a substance is the quotient of the mass m and its volume V

$$\rho = m/V \quad \text{SI units (kg/m}^3\text{)}$$

The relative density, D_4^{20} , of solids or liquids is the ratio between the mass of a volume of substance to be examined, determined at 20 °C, and the mass of the same volume of water, determined at 4 °C (at which temperature, water has its maximum density, i.e. 0.999975 kg/m³). The relative density has no dimension.

R.7.1.4.3 Test method(s)

Test methods for determining density are applicable to solids and liquids. [Table R.7.1-3](#) lists the respective test methods.

Table R.7.1-3 Test methods for determining density

Method	Applicability	Maximum Dynamic Viscosity (Liquids Only)/Pa.S
Hydrometer	Liquids	5
Hydrostatic balance	Solids and Liquids	5
Immersion ball	Liquids	20
Pycnometer	Solids and Liquids	500
Air comparison pycnometer	Solids	-
Oscillating densitometer	Liquids	5

EU Test guideline A3 for relative density (Regulation (EC) No 440/2008) includes a list of standards with technical information about the different methods and actual measuring of different types of substances.

R.7.1.4.4 Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

For liquids, it is useful to have some indication of the dynamic viscosity as this can affect the choice of method. The physical state of test substances should always be homogeneous, this is particularly relevant for highly viscous substances where internal bubbles can be formed; in these cases, the test substance should be allowed to rest until all internal bubbles have disappeared.

The study does not need to be conducted if:

- the substance is only stable in solution in a particular solvent and the solution density is similar to that of the solvent. In such cases, an indication of whether the solution density is higher or lower than the solvent density is sufficient; or
- the substance is gaseous at room temperature. In this case, an estimation based on calculation can be made from its molecular weight and the Ideal Gas Laws.

The summary should include the numerical value for density and temperature at which it was measured, test material identity, purity of the sample used, physical state, method and guideline used and reference substance (if any).

Waiving possibilities according to Annex XI to REACH

Use of existing data: Data on physical-chemical properties from experiments not carried out according to GLP or the test methods referred to in Article 13 (3) of REACH

The use of existing experimental data is possible if carried out by certified institutions.

Weight of evidence

Weight of evidence is normally not applicable.

(Q)SAR

(Q)SAR is generally not applicable for determination of relative density.

For this endpoint there are often experimental measurements and therefore QSPR models for this property have not received special attention in the environmental literature. Several software programs can be used to calculate the density of a given substance but the documentation and validation of the methods is limited.

Grouping of substances and read-across approach

Grouping and read across are normally not applicable.

Testing is technically not possible

Waiving relative density testing on the basis of not being technically possible is not applicable.

Further waiving possibilities

Not foreseen.

R.7.1.4.5 Impurities; uncertainties

Impurities can have a significant influence on the density. This influence depends on the amount and density of the impurity; thus, the higher the amount of impurity and the higher the difference between the densities of the main component and the impurity, the higher the influence. Care should be taken when using literature values as these are relevant for pure substances only (unless stated otherwise).

Density is temperature dependant. Whenever possible, determinations should be performed at 20 °C.

R.7.1.4.6 Endpoint specific information in the registration dossier / in IUCLID**Materials and methods**

- type of method or reference to the standard or the test method applied.

Results and discussion

- temperature (°C);
- relative density value (dimensionless);
- uncertainty in measurement.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on relative density can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual	ECHA Practical Guide N.3

			Chapter	
4.4	VII 7.4	Relative density	E.4.5	3.3

1

R.7.1.5 VAPOUR PRESSURE

R.7.1.5.1 Type of property

Vapour pressure is a property:

- for substance characterisation;
- which serves as a key parameter for assessing some toxicological and environmental hazards;
- which gives indications whether a substance may be available for inhalation as a vapour;
- which allows determining the volatility of a substance from an aqueous solution or soil.

R.7.1.5.2 Definition

The vapour pressure of a substance is defined as the saturation pressure above a solid or a liquid substance at constant temperature. At the thermodynamic equilibrium, the vapour pressure of a pure substance is a function of temperature only.

Note:

A substance which:

- (i) at 50 °C has a vapour pressure greater than 300 kPa (absolute); or
- (ii) is completely gaseous at 20 °C at a standard pressure of 101.3 kPa

is a gas according to the CLP Regulation.

R.7.1.5.3 Test method(s)

Method A.4 of Regulation EC 440/2008 or OECD Test Guideline 104 ('Vapour pressure') should be used for testing. It is useful to have preliminary information on the structure, the melting point and the boiling point of the substance to perform this test.

There is no single measurement procedure applicable to the entire range of vapour pressures. Therefore, several methods are recommended to be used for the measurement of vapour pressure from $< 10^{-4}$ to 10^5 Pa. For the selection of the test method the scope and applicability specifications have to be taken into account. The results should be checked for consistency with other physical data like boiling point, flash point etc.

It is recommended to determine the vapour pressure at least for two temperatures, for volatile substances (boiling point up to 150 °C) preferably at 20 °C and at 50 °C.

Where standards are applicable, the use of the most recent updates is advised, please check section R.7.1.1.3 for further information.

R.7.1.5.4 Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

Column 2 of REACH Annex VII provides the following specific rules for adaptation of the standard information requirement for vapour pressure:

The study does not need to be conducted if the melting point is above 300 °C.

If the melting point is between 200 °C and 300 °C, a limit value based on measurement or a recognised calculation method is sufficient.

Vapour pressure testing is also not required for substances with a standard boiling point of <30 °C, as these substances will have vapour pressures above the limit of measurement (i.e. 10⁵ Pa).

Waiving possibilities according to Annex XI to REACH

Use of existing data: Data on physical-chemical properties from experiments not carried out according to GLP or the test methods referred to in Article 13 (3) of REACH

The use of existing experimental data is possible if it has been determined by certified institutions. Further, the vapour pressure does not have to be determined experimentally if conclusive and consistent literature data are available.

Weight of evidence

For the determination of vapour pressure, weight of evidence is not possible.

(Q)SAR

For the determination of the vapour pressure, (Q)SAR approaches may be used if determination by experiment is not possible.

Grain (Grain, 1982) derived from thermodynamic principles two different estimation methods for vapour pressure that can be respectively applied for compounds that are liquid or gaseous at the temperature of interest (Equ. 7-1) and for solid and liquid compounds (Eq. 7-2). The first method is derived from the Antoine equation, which describes the temperature dependence of vapour pressure and it is formalised by the following equation:

$$\ln P_V = K_F (8.75 + R \ln T_b) (T_b - C)^2 / (0.97 RT) [1/(T_b - C) - 1/(T - C)]$$

(Equation 7-1)

where:

P_V = vapour pressure [atm] K_F = compound class specific constant

R = gas constant [cal/mol * K] T_b = boiling point [K]

T = environmental temperature [K] $C = -18 + 0.19 T_b$

The second method makes use of the Watson correlation, which describes the temperature dependence of the heat of vaporisation and it is quantified by this equation:

$$\ln P_V = K_F (8.75 + R \ln T_b) / (0.97 R) * [1 - (3 - 2T^*)^m / T^* - 2m(3 - 2T^*)^{m-1} \ln T^*]$$

(Equation 7-2)

where:

P_V = vapour pressure [atm] K_F = compound class specific constant

R = gas constant [cal/mol * K] T_b = boiling point [K]

T = environmental temperature [K] $T^* = T/T_b$

m = empirical factor depending on T^* and the physical state of the compound at the temperature of interest.

Liquids: $m = 0.19$

Solids: $T^* > 0.6$: $m = 0.36$

$0.6 > T^* > 0.5$: $m = 0.8$

$T^* < 0.5$: $m = 1.19$

The compound specific constant K_F is assumed to describe the polarity of the compound. K_F values are reported for simple compound classes by Grain (Grain, 1982) and its value varies between 0.97 and 1.23.

For compound classes not included in the tables, a K_F value of 1.06 is recommended. The factor K_F is derived for monofunctional compounds, but it is also applicable for polyfunctional compounds if assuming the respective highest K_F value.

A third method described by Mackay *et al.* (1982) is applicable only for hydrocarbons and halogenated hydrocarbons:

$$\ln P_V = - (4.4 + \ln T_b) (1.803 (T_b/T - 1) - 0.803 \ln (T_b/T) - 6.8 (T_m/T - 1))$$

where:

P_V = vapour pressure [atm] T_b = boiling point [K]

T_m = melting point [K] T = environmental temperature [K]

The OECD guideline 104 reports that the Watson correlation is applicable over the pressure range from 10^5 Pa to 10^{-5} Pa. It should in any case be pointed out that estimated values for vapour pressure can be subjected to great uncertainty if the computed pressure is lower than 1 Pa, especially when the boiling point has not been experimentally determined (OECD monograph 67). The uncertainty is even greater if the estimated value is used together with water solubility in order to estimate the Henry's Law constant.

The environment monograph 67 of the OECD describes all of the above mentioned methods and the OECD guideline 104 supports the use of the Watson correlation for the calculation of vapour pressure, but does not specifically reject other calculation methods.

The handbook for estimating the physico-chemical properties of organic compounds (Reinhard and Drefahl, 1999) reports another method based on thermodynamic properties and elaborated by Mishra and Yalkowsky that discussed the application of the method of Mackay (Mackay *et al.*, 1982).

The equation by Mishra and Yalkowsky gave significantly better estimates than the method of Mackay on the same data set (Mishra and Yalkowsky, 1991).

Another methodology that proved to be effective in estimating vapour pressure relies on group contribution approaches. Several models using this strategy have been proposed (Reinhard and Drefahl, 1999; see [Table R.7.1-4](#)).

Table R.7.1-4 Group contribution approach and vapour pressure

Compounds	Authors	Methodology	Statistics
Alkyl aromatic compounds	Amidon and Anik	Group contribution approach	Standard error ... 1.1 kJ on the estimation for the free energy of vaporisation
Mono-, di-, tri- and tetra substituted	Hoshino et al.	Group contribution approach	Average error 3.7 % Max. Error 30.9 %
Perfluorinated saturated hydrocarbons	Kelly et al.	Group contribution approach	Arithmetic mean deviation < 0.5 %

1

2 Numerous other models are available for the estimation of vapour pressure, and Grain (1990),
3 Schwarzenbach *et al* (1993), Delle Site (1996), Sage and Sage (2000) and Dearden (2003) have
4 reviewed many of these. The descriptors used in vapour pressure QSPRs include physico-chemical,
5 structural and topological descriptors, and group contributions. Katritzky *et al* (1998) used 4
6 CODESSA descriptors to model the vapour pressure (in atmospheres at 25°C) of 411 diverse
7 organic chemicals, with $r^2 = 0.949$ standard error = 0.331 log unit.

8 A number of studies (Andreev *et al* 1994, Kühne *et al* 1997, Yaffe & Cohen 2001) allow of the
9 estimation of vapour pressures over a range of temperatures.

10 **Grouping of substances and read-across approach**

11 For the determination of vapour pressure, read-across is not possible. Interpolation within
12 homologous series may however be used.

13 **Testing is technically not possible**

14 Vapour pressure testing is also not required for substances with a standard boiling point of < 30 °C,
15 as these substances will have vapour pressures above the limit of measurement (i.e. 10^5 Pa).

16 For substances which decompose during measurement or which are unstable or explosive in their
17 pure form, determination of the vapour pressure may not be technically possible. This also applies
18 to self-reactive substances and organic peroxides.

19 Pyrophoric substances may be difficult to handle experimentally. If fully inert conditions cannot be
20 maintained during sample preparation and measurement, use of an appropriate calculation method
21 is advised.

22 A calculation method should also be applied in the case of some corrosive substances which would
23 destroy essential metallic parts of the measurement apparatus.

24 Further waiving possibilities

25 Not foreseen.

26 **R.7.1.5.5 Impurities; uncertainties**

27 Impurities have a large influence on vapour pressure. The influence depends on the amount of the
28 impurity and its boiling point or volatility. Small amounts of volatile impurities may increase the

vapour pressure by several orders of magnitude. This has to be kept in mind when performing the measurements and for the interpretation of results.

Where there are volatile impurities in the sample which could affect the result, the substance may be purified. Test method A.4 states that it may also be appropriate to quote the vapour pressure for the technical material. However, in consideration of the large effect that impurities may have (see above), doing so is strongly discouraged.

R.7.1.5.6 Endpoint specific information in the registration dossier / in IUCLID

Materials and methods

- type of method or description of the apparatus or reference to the standard or the test method applied.

Results and discussion

- measured value of the vapour pressure for at least two temperatures;
- estimate of the vapour pressure at 20 or 25 °C;
- if a transition (change of state, decomposition) is observed, the following should be noted:
 - nature of change;
- temperature at which change occurs.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on vapour pressure can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.6	VII 7.5	Vapour pressure	E.4.7	3.5

R.7.1.5.7 References on vapour pressure

OECD Guidelines for the Testing of Chemicals / Section 1: Physical-Chemical properties, Test No. 104: Vapour Pressure, OECD Code: 979910401E1, July 2006.

Andreev N.N, Kuznetsov S.E, Storozhenko S.Y. (1994) Prediction of vapour pressure and boiling points of aliphatic compounds. Mendelev Comm. 173-174.

Grain C.F., (1982) Handbook of chemical property estimation methods. New York, Mc Graw-Hill

Delle Site A. (1996) The vapour pressure of environmentally significant organic chemicals: a review of methods and data at ambient temperature. J. Phys. Chem. Ref. Data 26:157-93.

Dearden JC. (2003) Quantitative structure-property relationships for prediction of boiling point, vapour pressure, and melting point. Environ Toxicol Chem 22(8):1696-709.

Katritzky AR, Y. W, Sild S, Tamm T, Karelson M. (1998) QSPR studies on vapour pressure, aqueous solubility, and the prediction of water-air partition coefficients. J. Chem. Inf. Comput. Sci. 38:720-5.

Kühne R, Ebert RU, Schüürmann G. (1997) Estimation of vapour pressures for hydrocarbons and halogenated hydrocarbons from chemical structure by a neural network. Chemosphere 34:671-86.

Mackay D, Bobra A, Chan W, Shiu WY. (1982) Vapour pressure correlation for Low-Volatility Environmental Chemicals. Environ. Sci. Technol. 16:645-9.

Mishra DS, Yalkowsky SH. Estimation of vapour pressure of some organic compounds. Ind. Eng. Chem. Res. 1991;30:1609-12.

OECD Guidelines for Testing of Chemicals, Method 104 “Vapour Pressure Curve”

Reinhard M, Drefahl (1999).A. Handbook for Estimating Physico-Chemical Properties of Organic Compounds. New York: Wiley.

Sage M.L, Sage G.W.(2000) Handbook of Property Estimation Methods for Chemicals. Boca Raton, FL: Lewis.

Schwartzenbach, R.P., Gswend, P.M., Imboden, D.M. (1993). Environmental Organic Chemistry. John Wiley and Sons.

Yaffe D, Cohen, Y (2001) Neural network based temperature-dependent quantitative structure property relationships (QSPRs) for predicting vapour pressure of hydrocarbons. J. Chem. Inf. Comput. Sci. 41:463-477.

R.7.1.6 SURFACE TENSION

R.7.1.6.1 Type of property

Surface tension is a non-classification related property. However, surface tension measurements of aqueous solutions are significant since decreasing the surface tension of water may impact on the properties of the solution and other physico-chemical measurements.

R.7.1.6.2 Definition

- Surface tension:

The free surface enthalpy per unit of surface area is referred to as surface tension (Council Regulation (EC) No 440/2008).

SI units for surface tension are N/m or mN/m. 1 N/m = 103 dynes/cm in historical units.

The surface tension of an aqueous solution of a substance can be used to determine whether the substance is surface active.

- Surface active substance (surfactant):

A surfactant is any organic substance and/or preparation used in detergents, which has surface-active properties and which consists of one or more hydrophilic and one or more hydrophobic groups of such a nature and size that it is capable of reducing the surface tension of water, and of forming spreading or adsorption monolayers at the water-air interface, and of forming emulsions and/or microemulsions and/or micelles, and of adsorption at water-solid interfaces (see Article 2 of Council Regulation (EC) No 648/2004).

R.7.1.6.3 Test method(s)

Testing should be done in accordance with one of the methods specified under section A.5 of the Test Methods Regulation ((EC) No 440/2008). These methods are applicable to most chemical substances.

It is useful to have preliminary information on the water solubility, the structure, the hydrolysis properties and the critical concentration for micelles formation of the substance before performing the test.

Surface tension measurements require a test material that is stable against hydrolysis during the test period and soluble in water at concentrations of >1 mg/l. Measurements should be performed on a solution at either 90 % of the solubility limit or 1 g/l, whichever is smaller.

R.7.1.6.4 Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

Column 2 of REACH Annex VII provides the following specific rules for adaptation of the standard information requirement for surface tension:

The study does not need to be conducted if:

- based on structure, surface activity is expected or can be predicted; or

- surface activity is a desired property of the material.

If the water solubility is below 1mg/l at 20 °C the test does not need to be conducted.

Waiving possibilities according to Annex XI to REACH

Use of existing data: Data on physical-chemical properties from experiments not carried out according to GLP or the test methods referred to in Article 13 (3) of REACH

As mentioned in Annex XI section 1.1.1. a number of conditions need to be met before such data can be used. Namely:

- (1) adequacy for the purpose of classification and/or risk assessment;
- (2) sufficient documentation is provided to assess the adequacy of the study; and
- (3) the data are valid for the endpoint being investigated and the study is performed using an acceptable level of quality assurance.

Weight of evidence

Not foreseen.

(Q)SAR

At the time of writing, no reliable (Q)SAR methods exist for sufficiently accurate predictions of surface tension.

The prediction of surface tension (σ) has been reviewed by Reinhard and Drefahl [1999] and Grain [1990]. Grain's recommended method, which is applicable to diverse chemical classes, is the Macleod-Sugden approach [Macleod 1923, Sugden 1924], which uses the following equation:

$$\sigma = (P\rho_L/M)^4$$

where P = parachor, ρ_L = liquid density, and M = molecular weight. Parachor is an easily calculated additive property, and Grain [1990] lists incremental P values for numerous atoms, groups and bonds. Reid et al [1977] found the Macleod-Sugden equation to yield a mean error in σ of 4.5 %.

If the density of the liquid is unknown, the method of Grain [1990] can be used:

$$\sigma = [(P/V_b)(1 + k)(3 - 2T/T_b)^n]^4$$

where k and n are constants listed by Grain [1990] for different chemical classes, V_b = molar volume at boiling point, T_b = boiling point (K). The method allows the calculation of surface tension at different temperatures, and has a mean error of 5.1 %.

Another approach to the calculation of surface tension at different temperatures is given by the Othmer equation:

$$\sigma(T) = \sigma_{\text{ref}} [(T_c - T)(T_c - T_{\text{ref}})]^{11/9}$$

where the subscript 'ref' refers to a reference temperature T_{ref} , and T_c = critical temperature. The parameters needed for the Othmer equation have been reported by Yaws et al [1991] for 633 chemicals.

Stanton and Jurs [1992], developed a 10-descriptor model for a set of 146 alkanes, esters and alcohols, and found a standard error of 0.4 dyne/cm. Kauffman and Jurs [2001] later developed a more general 8-descriptor model based on the viscosities of 213 common organic solvents.

Wang et al (2007) used both multiple linear regression and support vector machine (SVM) approaches to model the surface tension of 196 diverse pure liquid chemicals, using CODESSA descriptors. They found the SVM method better, with $R^2 = 0.93$.

Grouping of substances and read-across approach

At present grouping and read across are not applicable.

Testing is technically not possible

In this case testing should always be possible.

Further waiving possibilities

Not foreseen.

R.7.1.6.5 Impurities; uncertainties

For the measurement of surface tension the ring or plate tensiometer methods are preferred. The error on the measurement is in the order of 0.1–0.3 mN/m. Use of the standard protocols and GLP procedures are recommended. Surface active impurities in substances may in some cases lead to false-positive surface tension measurements.

R.7.1.6.6 Endpoint specific information in the registration dossier / in IUCLID

Materials and methods

- description of the apparatus and dimensions or reference to the standard or the test method applied;
- test material identity: apart from general issues, if surface tension of active impurities affects results, it should be noted.

Results and discussion

- surface tension value and unit (preferably mN/m or N/m but other units are also acceptable);
- concentration of the solution (as indicated in test A.5. Surface tension described in Council Regulation (EC) No 440/2008);
- age of solution;
- type of water or solution used;
- results from repeated measurements with varied equilibrium time (of the solution);
- Several measurement results should be provided to assess the possible timedependency of the measurement. Equilibration times may vary from minutes to hours. Measurements should be sufficient to prove that a constant surface tension was reached.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

1 ***Reference to other ECHA Guidance Documents***

2 Further detailed guidance on surface tension can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.10	VII 7.6	Surface tension	E.4.11	3.8

3
4 **R.7.1.6.7 References on surface tension**

- 5 ASTM D1331-89 (2001). Test methods for surface and interfacial tension of solutions of surface
6 active agents.
- 7 CEC (2004). Regulation (EC) No 648/2004 of the European Parliament and of the Council of 31
8 March 2004 on detergents. O.J. EU L104, 1-34.
- 9 CRC (2006). “Properties of Water in the Range 0 – 100°C”, in CRC Handbook of Chemistry and
10 Physics, 86th Edition, Taylor and Francis, Boca Raton, FL, 2006.
- 11 Elworthy, P.E. and K.J. Mysels (1966). The surface tension of sodium dodecyl sulfate solutions
12 and the phase separation model of micelle formation. J. Colloid Interface Sci. 21, 331-347.
- 13 EN (2004). I.S. EN 14370:2004. Surface active agents – Determination of surface tension.
- 14 Grain C.F. Surface tension. In Lyman W.J., Reehl W.F. and Rosenblatt D.H. (Eds.), Handbook of
15 Chemical Property Estimation Methods. American Chemical Society, Washington DC, 1990, pp.
16 20.1-20.16.
- 17 Hartland, S. (2004) Surface and Interfacial Tension - Measurement, Theory and Applications
18 Surfactant Science Series volume 199.
- 19 I.S. EN 14370:2004 (2004). Surface active agents – Determination of surface tension.
- 20 ISO (1985). ISO-304-1985 Surface active agents – Determination of surface tension by drawing
21 up liquid films.
- 22 Kauffman G.W. and Jurs P.C. Prediction of surface tension, viscosity, and thermal conductivity for
23 common organic solvents using quantitative structure-property relationships. J. Chem. Inf. Comput.
24 Sci. (2001) 41, 408-418.
- 25 Macleod D.B. On a relation between surface tension and density. Trans. Faraday Soc. (1923) 19,
26 38-42.
- 27 OECD (1995). OECD Guidelines for Testing of Chemicals, Method 115: Surface tension of
28 aqueous solutions, OECD, Paris.
- 29 Reinhard M. and Drefahl A. Handbook for Estimating Physicochemical Properties of Organic
30 Compounds. Wiley, New York, 1999.
- 31 Rosen, M.J. (2004) Surfactants and Interfacial Phenomena 3rd Ed. Wiley Interscience, New York,
32 NY USA.

- 1 Stanton D.T. and Jurs P.C. Computer-assisted study of the relationship between molecular structure
2 and surface tension of organic compounds. J. Chem. Inf. Comput. Sci. (1992) 32, 109-115.
- 3 Sugden S. The influence of the orientation of surface molecules on the surface tension of pure
4 liquids. J. Chem. Soc. (1924) 125, 1167-1189.
- 5 Tolls, J. and Sijm, D.T.H.M. (2000). Estimating the properties of surface active chemicals. In: R.S.
6 Boethling and D. Mackay, eds. Handbook of Environmental and Health Sciences; Property
7 Estimation Methods for Chemicals.
- 8 Wang, J., Du H., Liu H., Yao X., Hu Z. and Fan B. Prediction of surface tension for common
9 compounds using heuristic method and support vector machine. Talanta (2007) 73, 147-156.
- 10 Yaws C.L., Yang H.-C. and Pan X. 633 Organic chemicals: surface tension data. Chem. Eng.
11 (1991) March, 140-150.
- 12

R.7.1.7 WATER SOLUBILITY

R.7.1.7.1 Type of property

Water solubility is a significant parameter for a number of reasons:

- The mobility of a test substance is largely determined by its solubility in water. In general, highly soluble substances are more likely to be distributed by the hydrological cycle.
- It can affect adsorption and desorption on soils and volatility from aquatic systems. Substances that are highly water soluble are more likely to desorb from soils and less likely to volatilise from water. Water solubility can also affect possible transformations by hydrolysis, photolysis, oxidation and reduction.
- Water soluble substances gain access to humans and other living organisms. Water solubility has a significant impact on the bioavailability of a compound as well as their general ADME properties.
- Knowledge of the water solubility is a prerequisite for setting up test conditions for a range of fate (e.g. biodegradation, bioaccumulation) and effects studies.
- It is also used to derive other environmental parameters, such as K_{ow} , K_{oc} and Henry's Law Constant.

R.7.1.7.2 Definition

The solubility of a substance in water is specified by the saturation mass concentration of the substance in water at a given temperature. The solubility in water is specified in units of mass per volume of solution. The SI unit is kg/m^3 (grams per litre may also be used).

Mixtures of organic compounds, e.g. petroleum substances, behave differently from their single constituent compounds when brought into contact with water. Petroleum substances are typically hydrophobic and exhibit low solubility in water. However, reflecting the range of structures, constituent hydrocarbons will exhibit a wide range of water solubility. Therefore, water solubility measurements for these substances are loading rate dependent due to their complex composition. This water solubility behaviour impacts on both the conduct and interpretation of aquatic toxicity tests for these complex substances. The complex composition, and generally low water solubility, impact also on the choice and conduct of biodegradation studies.

The same testing issues also apply to inorganic compounds. Solubility of metal compounds will depend on the species, the particle size and the characteristics of the aqueous medium. As with petroleum products, the solubility properties of a given complex substance can differ substantially from the individual constituents.

Consequently, the above definition for solubility of a single substance in water is not applicable to substances which are multi-component, such as multi-constituent or UVCB substances, i.e. complex substances. The usually accepted meaning of *solubility* in such cases is *the composition of the aqueous solution formed at equilibrium under a defined set of conditions*. Temperature and the amount of substance added per unit volume of water (i.e. the *loading*) are the main factors to consider. It may not always be possible to establish that equilibrium of all components has been achieved; in these cases, time and type of agitation of the test vessels must also be described.

1 R.7.1.7.3 Test method(s)

2 No single method is available to cover the whole range of solubilities in water, from relatively
3 soluble to very low soluble substances. General test guidelines (OECD Method 104; EU Method
4 A6) include two test methods which cover the whole range of solubilities but are not applicable to
5 volatile substances. Water solubility determinations are normally run at 20 °C in distilled water
6 according to standard test guidelines (OECD Method 104; EU Method A6). Solubility data
7 determined using these standard physico-chemical guidelines may differ if the test material is
8 solubilised in either aqueous solutions containing salts or at different test temperatures (or both)
9 (e.g. ecotoxicological test media).

10 The methods should be applied to essentially pure substances that are stable in water. Details of
11 suitable methods are shown in Table R.7.1-5.

12 A number of standardised methods are available for the determination of single substances and
13 complex mixtures of liquids and solids. The test methods are not applicable to volatile substances.
14 Care should be taken to ensure that the test substances examined are as pure as possible and their
15 solubility levels are determined analytically using a specific analytical method wherever possible.
16 Precautions should be taken to minimise degradation of the test substance, in particular if long
17 periods of equilibration are required (e.g. *slow stir* methods).

18 Measurement of water solubility does not usually impose excessive demands on chemical
19 techniques. However, measurement of the solubility of sparingly soluble compounds requires
20 extreme care to generate saturated solutions of the material without the introduction of dispersed
21 material; invariably specific methods of analysis are able to determine the low levels (sub ppb-ppm)
22 in solution. Reported water solubility data for such compounds can often contain appreciable errors.

Table R.7.1-5 Test methods for the determination of water solubility

Method details	Applications and requirements	Repeatability and sensitivity
<p>Column elution method</p> <p>Based on elution of the test substance with water from a micro-column which is charged with an inert carrier material such as glass beads, silica gel or sand and an excess of test substance. The water solubility is determined when the mass concentration of the eluate is constant.</p> <p>The mass concentration of the test substance is determined analytically</p>	<p>Applicable to essentially pure substances only</p> <p>Used for low solubilities ($< 10^{-2}$ g/l)</p> <p>Organic substances, but not mobile oils or liquids</p>	<p>$< 30 \%$; down to $1 \mu\text{g/l}$</p>
<p>Flask method</p> <p>The test substance is dissolved in water at a temperature somewhat above the test temperature. When saturation is achieved the mixture is cooled and kept at the test temperature, stirring as long as necessary to reach equilibrium</p> <p>The mass concentration of the test substance is determined analytically</p>	<p>Applicable to essentially pure substances and also complex substances.</p> <p>Use of fast stirring techniques (300-400 rpm) appropriate for higher solubility ($> 10^{-2}$ g/l) test substances.</p> <p>Use of slow-stirring techniques (< 100 rpm) appropriate for low solubility ($< 10^{-2}$ g/l) test substances (Letinski et al, 2002)</p> <p>Requires equilibration study to determine the time taken to equilibrate the test substance and water</p>	<p>$< 15 \%$; down to $1 \mu\text{g/l}$</p>

R.7.1.7.4 Adaptation of the standard testing regimeWaiving possibilities according to column 2 of Annex VII to REACH

Column 2 of REACH Annex VII provides the following specific rules for adaptation of the standard information requirement for water solubility:

The study does not need to be conducted if:

- *the substance is hydrolytically unstable at pH 4, 7 and 9 (half-life less than 12 hours); or*
- *the substance is readily oxidisable in water; or*
- *the substance is flammable in contact with water.*

If the substance appears 'insoluble' in water, a limit test up to the detection limit of the analytical method shall be performed.

For ionising substances, the pH-dependence of the water solubility should be known. At least the pH of the test water needs to be identified. In the context of marine risk assessment, when the pK_a is close to 8 it may be necessary to obtain realistic measurements using seawater.

For volatile compounds, it can be useful to have information on the vapour pressure.

Waiving possibilities according to Annex XI to REACH

Use of existing data: Data on physical-chemical properties from experiments not carried out according to GLP or the test methods referred to in Article 13 (3) of REACH

Most physical properties, such as molecular weight, melting point, boiling point, density and water solubility can be obtained from commonly used environmental Handbooks, such as Verschueren's Handbook of Environmental Data on Organic Chemicals (1983), Howard's Handbook of Environmental Fate and Exposure Data, Vol. I and II (1990), Lide's CRC Handbook of Physics and Chemistry, Lange's Handbook of Chemistry, the Merck Index, the Aldrich Catalog, Kirk-Othmer Encyclopaedia of Chemical Technology and other handbook compilations such as Riddick *et al.* (1986).

Alternatively, searching on various environmental databases, such as HSDB (<http://www.toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>), will provide summaries of chemical and physical properties of substances.

It is not unusual to find in the literature a wide range of solubilities for the same product. The oldest literature generally yields the highest solubility values: this is due to the fact that products were originally not as pure as they are nowadays and also non-specific methods were used which would not differentiate between the dissolved product and any impurities. Reported water solubility data for such compounds can often contain appreciable errors. Therefore, the reliability of data must be demonstrated by providing information on the identity and purity of the test substance, the methodology used to make the measurement, and whether or not this was performed to GLP standards.

Weight of evidence

Secondary data sources can be used in a Weight of Evidence approach and they can collectively support the choice of a specific value for the water solubility. These secondary sources have to be based on a critical evaluation of peer-reviewed data and a consequent selection of a reliable and representative value for the water solubility. The use of Klimisch codes, can be extended to these secondary sources and a reliability code of (2) *valid with restrictions* should be assigned when using an authoritative secondary source.

A number of standardised methods are available for the determination of single substances and complex mixtures of liquids and solids. The test methods are not applicable to volatile substances. Care should be taken to ensure that the test substances examined are as pure as possible and their solubility levels are determined analytically using a specific analytical method wherever possible. Precautions should be taken to minimise degradation of the test substance, in particular if long periods of equilibration are required (e.g. *slow stir* methods).

Measurement of water solubility does not usually impose excessive demands on chemical techniques. However, measurement of the solubility of sparingly soluble compounds requires

extreme care to generate saturated solutions of the material without the introduction of dispersed material; invariably specific methods of analysis are able to determine the low levels (sub ppb-ppm) in solution. Reported water solubility data for such compounds can often contain appreciable errors.

(Q)SAR

At present (Q)SAR is generally not applicable for determination of water solubility.

Water solubility depends not only on the affinity of a solute for water, but also on its affinity for its own crystal structure. Molecules that are strongly bound in their crystal lattice require considerable energy to remove them. This also means that such compounds have high melting points, and in general high-melting compounds have poor solubility in any solvent.

Removal of a molecule from its crystal lattice means an increase in entropy, and this can be difficult to model accurately. For this reason, as well as the fact that the experimental error on solubility measurements can be quite high (generally reckoned to be about 0.5 log unit), the prediction of aqueous solubility is not as accurate as is the prediction of partition coefficient. Nevertheless, many papers (Dearden 2006) and a book (Yalkowsky & Banerjee 1992) have been published on the prediction of aqueous solubility, as well as a number of reviews (Lyman 1990, ECETOC 1998, Reinhard & Drefahl 1999, Mackay 2000, Schwarzenbach *et al* 2003, Dearden 2006). There are also a number of software programs available for that purpose (ECETOC 2003, Dearden 2006). Livingstone (2003) has discussed the reliability of aqueous solubility predictions from both QSPRs and commercial software.

It should be noted that there are various ways that water solubilities can be reported: in pure water, at a specified pH, at a specified ionic strength, as the undissociated species (intrinsic solubility), or in the presence of other solvents or solutes. Solubilities are also reported in different units, for example g/100 ml, mole/litre, mole fraction. The use of mole/litre is recommended, as this provides a good basis for comparison.

For solids, work has to be done to remove molecules from their crystal lattice, and the simplest way to account for this is to use what Yalkowsky and co-workers have termed the general solubility equation (GSE), which incorporates a melting point term to account for the behaviour of solids (Sanghvi *et al* 2003):

$$\log S_{\text{aq}} = 0.5 - \log K_{\text{ow}} - 0.01(\text{MP} - 25)$$

where MP is the melting point (°C). The melting point term is taken as zero for compounds melting at or below 25°C. Calculated log K_{ow} and MP values can be used in the GSE, although measured values are preferred. Aqueous solubilities of 1026 non-electrolytes, with a log S_{aq} range of -13 to +1 (S in mole L⁻¹), calculated with the GSE had a standard error of 0.38 log unit.

Good predictions for a large diverse data set have been obtained by the use of linear solvation energy descriptors (Abraham & Le 1999):

$$\log S_{\text{aq}} = 0.518 - 1.004 R + 0.771 \pi^{\text{H}} + 2.168 \Sigma\alpha^{\text{H}} + 4.238 \Sigma\beta^{\text{H}} - 3.362 \Sigma\alpha^{\text{H}}.\Sigma\beta^{\text{H}} \\ - 3.987 V_{\text{X}}$$

$$n = 659 \quad r^2 = 0.920 \quad s = 0.557$$

where R = excess molar refractivity (a measure of polarisability), π^{H} = a polarity/polarisability term, $\Sigma\alpha^{\text{H}}$ and $\Sigma\beta^{\text{H}}$ = sums of hydrogen bond donor and acceptor abilities respectively, and V_{X} = McGowan characteristic molecular volume. Because the Abraham descriptors are approximately

auto-scaled, it can be seen from the Abraham and Le equation that the main factors controlling aqueous solubility are hydrogen bond acceptor ability and molecular size.

Solubility can vary considerably with temperature, and it is important that solubility data are reported at a given temperature.

Grouping of substances and read-across approach

At present grouping and read across are not applicable.

Testing is technically not possible

For this endpoint, testing should almost always be possible and water solubility should usually be determined experimentally. If it is technically not possible to conduct the study as a consequence of the properties of the substance (e.g. substances flammable in contact with water or substances readily oxidisable in water), testing may be omitted according to general rules for adaptation of the standard testing regime described in REACH Annex XI, Section 2.

Further waiving possibilities

Not foreseen.

R.7.1.7.5 Impurities; uncertainties

The water solubility of the test substance can be considerably affected by the presence of impurities.

For a complex substance, the measured solubility is dependent on the amount of test substance added. In practical terms, solubility data are generated using at least two loading rates (e.g. 100 mg/l and 1000 mg/l). Accuracy in determining water solubility decreases as the water solubility of a test substance is reduced (e.g. as shown for reference substance data in OECD Method 105). When dealing with test substances with water solubilities of the order of <10 µg/l, precautions need to be taken to avoid the introduction of dispersed material into the final extract.

R.7.1.7.6 Endpoint specific information in the registration dossier / in IUCLID

Materials and methods

- description of the apparatus and dimensions or reference to the standard or the test method applied;
- results from preliminary test (if any);
- chemical identity and impurities (preliminary purification step, if any);
- water temperature during saturation process;
- analytical method employed;
- any evidence of chemical instability;
- all information relevant for the interpretation of the results.

If Column Elution method:

- concentrations, flow rates and pH for each sample;
- mean and standard deviations of five samples at least;
- average for each of two successive runs at least;
- nature and loading of support material;
- solvent used.

If Flask method:

- pH of each sample;

- individual analytical determinations and the average;
- average of the values for different flasks.

Results and discussion & Applicant's summary and conclusion

- water solubility in (mg/L) at temperature (°C);
- pH value and concentration of test substance;
- pKa value at 25 °C;
- description of solubility (if relevant).

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on water solubility can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.8	VII 7.7	Water solubility	E.4.9	3.7

R.7.1.7.7 References on water solubility

- Abraham M.H. and Le J. (1999) The correlation and prediction of the solubility of compounds in water using an amended solvation energy relationship. *J. Pharm. Sci.* 88, 868-880.
- Dearden J.C. (2006) *In silico* prediction of aqueous solubility. *Expert Opinion on Drug Discovery* 1, 31-52.
- EC Method A6. "Water Solubility", Dir 92/69/EEC, Official Journal of the European Communities, O.J. L383 A)
- EC Method A7. "Hydrolysis ", Dir 92/69/EEC, Official Journal of the European Communities, O.J. L383 A)
- ECETOC Technical Report No. 74: *QSARs in the Assessment of the Environmental Fate and Effects of Chemicals*. ECETOC, Brussels, 1998.
- ECETOC Technical Report No. 89: *(Q)SARs: Evaluation of the Commercially Available Software for Human Health and Environmental Endpoints with Respect to Chemical Management Applications*. ECETOC, Brussels, 2003.
- Livingstone D.J. (2003) Theoretical property predictions. *Current Topics in Med. Chem.* 3, 1171-1192.
- Mackay D. Solubility in water. In Boethling R.S. and Mackay D. (Eds.), *Handbook of Property Estimation Methods for Chemicals: Environmental and Health Sciences*. Lewis, Boca Raton, FL, 2000, pp. 125-139.
- OECD Environmental Health and Safety Publications, 2000. Number 23. Guidance document on aquatic toxicity testing of difficult substances and mixtures.
- OECD Environment, Health and Safety Publications, 2001. Series on Testing and Assessment, No. 29, Guidance Document on Transformation/Dissolution of Metals and Metal Compounds in Aqueous Media
- OECD Guidelines for Testing of Chemicals – Method 105 "Water Solubility"
- OECD Guidelines for Testing of Chemicals – Method 111 "Hydrolysis as a Function of pH"
- Reinhard M. and Drefahl A. Handbook for Estimating Physico-chemical Properties of Organic Compounds. Wiley, New York, 1999.
- Sanghvi T., Jain N., Yang G. and Yalkowsky S.H. (2003) Estimation of aqueous solubility by the general solubility equation (GSE) the easy way. *QSAR Comb. Sci.* 22, 258-262.
- Schwarzenbach R.P., Gschwend P.M. and Imboden D.M. (2003) *Environmental Organic Chemistry*, 2nd edition, Wiley, Hoboken, NJ.
- Yalkowsky S.H. and Banerjee S. (1992). Aqueous Solubility: Methods of Estimation for Organic Compounds. Marcel Dekker, New York.

R.7.1.8 PARTITION COEFFICIENT N-OCTANOL/WATER**R.7.1.8.1 Type of property**

The n-octanol/water partition coefficient (K_{ow}) is one of the key physico-chemical parameters, and it is used in numerous estimation models and algorithms for environmental partitioning, sorption, bioavailability, bioconcentration, bioaccumulation and also human toxicity and ecotoxicity. As such K_{ow} is a critical parameter for chemical safety assessment, classification and labelling, and PBT assessment.

The generation of a K_{ow} value is required at all tonnage bands (i.e. > 1 t/y; information requirements according to REACH Annexes VII-X).

R.7.1.8.2 Definition

The n-octanol/water partition coefficient (K_{ow}) is defined as the ratio of the equilibrium concentrations of a dissolved substance in a two-phase system consisting of the largely immiscible solvents n-octanol and water. The property is moderately temperature-dependent and typically measured at 25 °C.

R.7.1.8.3 Test method(s)

EU test guideline A.8 describes two direct measurement methods; the Shake Flask method (OECD 107) and the HPLC method (OECD 117). The Shake Flask method falls within the logKow range -2 to 4 and the HPLC method within the range 0 to 6. The applicability of the methods differs depending on the substance type and the amount of impurities in the test substance. Neither of the methods is applicable to surface active materials, for which a calculated value or an estimate based on individual solubilities should be provided.

Regardless of the method used, highly accurate measurements of log K_{ow} >~5 are complicated by the fact that small amounts of octanol are entrained in the aqueous phase, leading to a potential underestimation of the measured log K_{ow} values. All of the direct methods for measuring log K_{ow} require quantifying the test material in either octanol or water and preferably in both matrices.

In addition, the OECD test guidelines (123, Slow-stirring method; and 122, pH-Metric Method for Ionisable Substances, draft) can be used to generate data for this endpoint provided that a sufficient justification for the use of these methods is reported.

1 **Table R.7.1-6 Methods for determination of partition coefficient n-octanol/water**

Method details	REPEATABILITY	APPLICABILITY RANGE
<p>Shake Flask Method (EU A.8, OECD 107)</p> <p>The Shake Flask method is the default procedure. It is considered to give accurate results for low to medium hydrophobic substances. For substances with a high expected $\log K_{ow}$, alternative methods are recommended. A suitable analytical method is needed to determine the concentration of the test material in the octanol and water phases. By applying mass balance considerations, it may be possible to measure the test material in only the less-soluble phase. However, this approach significantly decreases the reliability in the reported value.</p> <p>This technique is not suitable for surface active compounds (surfactants), or compounds that hydrolyse rapidly.</p>	Three replicates should fall within $\pm 0.3 \log K_{ow}$	$-2 < \log K_{ow} < 4$
<p>HPLC Method (EU A.8, OECD 117)</p> <p>This is a relatively quick way of estimating $\log K_{ow}$. It is not measured directly, but from a correlation between $\log k$ (capacity factor) and $\log K_{ow}$ for a series of reference substances. It therefore depends on the quality of the $\log K_{ow}$ measurement of reference substances (often measured by the shake flask method). A series of reference compounds with similar chemical functionality to the test material should be used to generate the $\log k$: $\log K_{ow}$ correlation. In general, the HPLC method is less sensitive to impurities than the shake flask method. The RP-HPLC is not recommended for strong acids and bases, metal complexes or surface active agents, or for measurements across very different classes of substances. The HPLC method is also very suitable for measuring the K_{ow} of mixtures of chemical homologues.</p>	Three replicates should fall within $\pm 0.1 \log K_{ow}$	$0 < \log K_{ow} < 6$
<p>Slow-Stirring Method (OECD 123)</p> <p>This is a more recent method developed as an alternative to the shake flask procedure (OECD 107, EU A.8). The advantage of slow stirring versus shaking is that emulsion formation will be reduced. The method requires a few days to reach equilibrium. The method may be difficult to adapt to a high throughput approach. As with the other direct</p>	Intralaboratory median standard deviation from $0.15 - 0.3 \log K_{ow}$ (Tolls et al, 2003).	Validation has shown that this method can also be used for very hydrophobic substances, up to $\log K_{ow}$ 8.3 (OECD 2003, Tolls et al, 2003).

<p>methods, a suitable analytical method is needed to measure the concentration of the test material in the octanol and water phases.</p> <p>NB: Radiolabelled substances – which may be synthesised for use in other tests – can be very useful for accurate log K_{ow} determination.</p>		
<p>Computational Approach in OECD Guideline 107 (EU A.8)</p> <p>This method enables partition coefficients to be calculated based on the ratio of the solubility of the material in octanol and water. For some substances (e.g. some surfactants and pigments) it is technically not feasible (or good practice) to measure an octanol-water partition coefficient by OECD 107, and other methods (OECD 117 and QSAR) may be unsuitable as they are based on extrapolations of measured values. For such substances it may be possible to obtain a ratio of the saturated water solubility (OECD 105) and saturated octanol solubility (no guideline currently available but based on the principles of OECD 105). The calculation method however has the drawback that it does not include the interaction between the water and solvent phase (i.e. a substance with high K_{ow} is rather 'pushed out of the water' than 'pulled into octanol'). This explains the poor correlation typically observed between octanol solubility and K_{ow} (Dearden, 1990, Sijm et al., 1999). The ratio was found to be somewhat more representative if one uses octanol/saturated water and water/saturated octanol.</p> <p>As such, a ratio calculation would be a less preferred yet acceptable alternative for the octanol/water partition coefficient (K_{ow}), but must be treated with caution as it would not have been derived in the same manner as other K_{ows} (OECD 107).</p>		

1

2 R.7.1.8.4 Adaptation of the standard testing regime

3 If experimental testing is not possible, log K_{ow} must be estimated by an appropriate *in silico* method
4 based on the molecule's structure. A computational (*in silico*) method shall be used in case the test
5 cannot be technically performed. This can be the case for example if the substance decomposes, has
6 a high surface activity, reacts violently during the performance of the test, or does not sufficiently
7 dissolve in water or in octanol, or if it is not possible to obtain a sufficiently pure substance.

Waiving possibilities according to column 2 of Annex VII to REACH

K_{ow} does not need to be determined if the substance is purely inorganic. In addition, if the testing is technically not possible (e.g. substance decomposes, has a high surface activity, reacts violently during the performance of the test, does not sufficiently dissolve in water or in octanol, or if it is not possible to obtain a sufficiently pure substance), it can be waived. In these cases, a calculated value of $\log K_{ow}$ as well as the details of the calculation should be provided. In case of reaction with water the properties of the degradation products have to be included in the PBT assessment and thus information on the K_{ow} of the relevant degradation products has to be generated and reported in the dossier.

Waiving possibilities according to Annex XI to REACH

The reporting of the K_{ow} information cannot usually be waived because it is essential for CSA, classification and labelling and PBT assessments.

Use of existing data: Data on physical-chemical properties from experiments not carried out according to GLP or the test methods referred to in Article 13 (3) of REACH

(Measured) $\log K_{ow}$ is a commonly documented property in substance databases, such as IUCLID (<http://ecb.jrc.it>), or MedChem (<http://www.daylight.com>) which includes approximately 61,000 measured $\log K_{ow}$ values. The PHYSPROP database of the Syracuse Research Corporation contains $\log K_{ow}$ data for over 25000 substances (<http://www.syrres.com>). Additional sources are the Canadian National Committee for CODATA (CNC/CODATA) database with evaluated $\log K_{ow}$ values for over 20000 substances (<http://logKow/cisti/nrc/ca>) and the QSAR Toolbox programme (<http://www.qsartoolbox.org>), which provides calculated $\log K_{ow}$ values and experimental values if available.

Weight of evidence

Measured values are given precedence over calculated values. For organic substances experimentally derived high-quality K_{ow} values, or values which are evaluated in reviews and assigned *recommended values*, are preferred over other determinations of K_{ow} .

(Q)SAR

When no experimental data of high quality are available, or if experimental methods are known to be unreliable, valid (Q)SARs for $\log K_{ow}$ may be used. Such valid (Q)SAR models may be used if they are restricted to substances for which their applicability is well characterised.

Many publications have dealt with the estimation of $\log K_{ow}$ values from molecular structure, and Lyman (1990), Schwarzenbach *et al* (1993), Nendza (1998), Reinhard and Drefahl (1999), Leo (2000), Livingstone (2003) and Klopman and Zhu (2005) have reviewed prediction methods for $\log K_{ow}$; Livingstone (2003) in particular gives a detailed critical analysis of available methods. The main prediction methodologies are based on physico-chemical, structural and/or topological descriptors or on atomic or group contributions. For example, Bodor *et al* (1989) developed a QSPR with 14 physico-chemical and quantum chemical descriptors to model $\log K_{ow}$ of a diverse set of 118 organic chemicals, with $r^2 = 0.882$ and a standard error of 0.296 log unit. The method of Ghose *et al* (1988) used atomic contributions, and on a set of 893 compounds the standard error was 0.496 log unit. Klopman and Wang (1991) used their MCASE group contribution approach to predict the $\log K_{ow}$ values of 935 organic compounds with a standard error of 0.39 log unit. This error is close to the experimental error on $\log K_{ow}$.

A method of predicting log K_{ow} values that provides mechanistic insight is that of Abraham *et al* (1994). Using their solvatochromic descriptors they developed the following QSPR:

$$\log K_{ow} = 0.088 + 0.562 R - 1.054 \pi^H + 0.034 \Sigma\alpha^H - 3.460 \Sigma\beta^H + 3.814 V_x$$

$$n = 613 \quad r^2 = 0.995 \quad s = 0.116$$

where R = excess molar refractivity, π^H = a polarity term, $\Sigma\alpha^H$ and $\Sigma\beta^H$ = hydrogen bond donor and acceptor abilities respectively, and V_x = the McGowan characteristic molecular volume. Since the descriptors are approximately autoscaled, the magnitudes of the coefficients give an indication of the relative contribution of each descriptor to log K_{ow} . Thus it can be seen that hydrogen bond acceptor ability and molecular size make the most important contributions to log K_{ow} ; on the other hand the contribution of hydrogen bond donor ability is negligible, and this is attributed to the hydrogen bond acceptor abilities of both water and octanol being very similar, while in contrast the hydrogen bond donor ability of water is very strong, accounting for the high negative coefficient on the $\Sigma\beta^H$ term. The standard error is very low, and may indicate some over-fitting of the data.

There are also numerous software programs⁹ available for the estimation of Log K_{ow} of organic substances, and some of these give good predictions. A recent comparison of 14 such programs (Dearden *et al* 2003) found that, using a 138-substance test set, the percentage of substances with log K_{ow} predicted within +/-0.5 log unit of the measured log K_{ow} value ranged from 94 % to 50 %.

It is important to point out that, contrary to what might be thought, solubility in octanol is of no value as a measure of lipophilicity. When a chemical is taken up by lipid *in vivo*, it is always from an aqueous phase, and so it is the distribution between aqueous and lipid phases that is important, and not the absolute solubility in lipid. In fact, the term hydrophobicity is preferable to lipophilicity, because the driving force for transfer from water to lipid comes largely from the aqueous phase; that is, a chemical is pushed from water to lipid, rather than being pulled by lipid from water. The driving force has a large entropic component (Dearden & Bresnen 2005) because of water-structuring. Octanol tends to behave much as an ideal solvent, and solubility in octanol (S_o) is inversely correlated with melting point, but not with octanol-water partition coefficient. Dearden (1990) showed that the correlation between log K_{ow} and log S_o is very poor.

It is also pointed out that the calculation of log K_{ow} from the ratio of solubilities in octanol and water is rather inaccurate, as the results below show (Yalkowsky *et al* 1983):

Solute	log (S_o/S_w)	log K_{ow}
Antipyrine	-0.73	0.26
Ethyl 4-aminobenzoate	1.86	1.96
Caffeine	-0.75	-0.20
Theophylline	-0.57	-0.09

⁹ It should be noted that a calculated log K_{ow} value relates to the unionised form of a chemical. Some software will also calculate log D_{ow} , where D_{ow} is the distribution coefficient taking into account both ionised and unionised species; this requires a knowledge of pKa, which the software also calculates. log D_{ow} is related to Log K_{ow} as follows:

For acids: $\log D_{ow} = \log K_{ow} - \log(1 + 10^{(pH-pKa)})$

For bases: $\log D_{ow} = \log K_{ow} - \log(1 + 10^{(pH-pKa)})$

1 **Grouping of substances and read-across approach**

2 At present grouping and read across are not applicable.

3 **Testing is technically not possible**

4 In this case testing should always be possible.

5 Further waiving possibilities

6 Not foreseen.

7 **R.7.1.8.5 Impurities; uncertainties**

8 The effect of impurities in the test substance are discussed in the referenced test guidelines.

9 Difficult to test substances:

10 There are certain structural or physico-chemical properties that can make the accurate determination
11 of K_{ow} or its measurement difficult. Difficult to test substances include poorly soluble, volatile,
12 surface active, ionisable substances, mixtures of substances, as well as substances subject to rapid
13 degradation due to such processes as phototransformation, hydrolysis, oxidation, or biotic
14 degradation.

15

16 Guidance on regulatory compliant K_{ow} determination for ionisable substances and salts:

17

18 The K_{ow} is typically defined as the partition coefficient of the neutral, undissociated form of a
19 substance. However, the relative extent to which an ionisable substance is likely to be dissociated in
20 the environment (with pH usually in the range 5-9) can have a marked effect on its physicochemical
21 properties, especially the octanol-water partition coefficient and water solubility, which in turn
22 affect fate and behaviour. As log K_{ow} is routinely used to predict bioconcentration/bioaccumulation
23 potential, this aspect is especially important in a PBT context. For substances which dissociate
24 within an environmentally relevant pH range (pKa 5-9), values for K_{ow} must be derived for the
25 neutral form, and preferably also for the dissociated form. In some cases a factor 4-5 has been
26 recorded between the log K_{ow} of both species. The value for the dissociated molecule determined
27 around a pH of 7 (sometimes referred to as D_{ow}) is considered more realistic for PBT and chemical
28 safety assessment.

29

30 Based on practical experience the following guidance is provided:

31

32 *Simple acids and bases in the normal pH range:*

- 33 o The HPLC method is to be applied to acids and bases in their non-ionised forms, although
- 34 the pH should be kept in the range 2 to 9 (however pH 5 to 9 is preferred).
- 35 o For the shake-flask method, the approach must be followed in which the study is
- 36 conducted at a pH where the substance is not ionised, if possible, or at a pH where the extent
- 37 of ionisation is minimised.
- 38 o Validated QSAR estimations may be useful for acids and bases.

39

40 *Zwitterionic substances:*

- 41 o For zwitterions, the shake-flask method should be used to develop a valid K_{ow} value. Even
- 42 if the ionic charge pattern of the compound in octanol is not known, the value represents a
- 43 practical and useful parameter. It is not justifiable to expect a full description of all the
- 44 equilibria in both water and octanol. The pH of such a study should be 7 or the iso-electric

point, as long as that point is in the range pH 5 to 9, so as to maximise the possibility of partition into octanol. There is no need to give both pH values.

o The HPLC method must not be used. The usual estimation methods should be valid, but particular care should be exercised.

o QSAR estimations may be useful provided that they are validated.

Salts of organic compounds:

o The shake-flask method should be used, usually at pH 7, or at any pH in the range 5 to 9 which maximises the potential for partition into octanol. For salts, the nature of the analytical method compared to the chemical composition will have to be considered. The ideal is to monitor cation and anion** individually in both phases. When only one half can be analysed, then the result must be understood as partial, even if it is the best that is achievable.

o Estimation by HPLC is not valid for the whole salt.

o QSAR methods will be valuable in assessing the properties of each half of the salt. Current estimation methods cannot estimate the K_{ow} of the ion pair.

Guidance on regulatory compliant K_{ow} determination for surfactants:

In many cases a calculated K_{ow} value will be the first choice for surfactants. It is also useful to compare a calculated with a measured value. For the calculation approaches, one needs to consider the pH of the system (which determines the ionisation of the surfactant – see Section R.7.1.17). None of the experimental methods is very well suited for determining the K_{ow} of surface active substances. The shake flask method is the least suitable experimental method for surfactants. HPLC methodology may fail due to secondary interactions, and is sensitive to fluctuations of ionic strength. The slow stirring method in theory is the best, but still not demonstrated to be perfect. If using slow stir, one needs to demonstrate a consistent result when starting with the surfactant in either phase, not just in the octanol. Another approach for surfactants can be the comparison of measured solubilities in octanol and water. However, it is prudent to take the critical micelle concentration in water (CMC) as a solubility limit, in order to avoid unrealistically low K_{ow} values.

Guidance on regulatory compliant K_{ow} determination for mixtures:

It is possible that different components of mixtures have significantly different behaviour in the physico-chemical tests and therefore also *in vivo* and in the environment. It is therefore important to ensure that the results presented for the physico-chemical tests represent each component rather than the mixture being treated as a single component. For simple mixtures where the components are known and easily identifiable, this may mean presenting individual values for K_{ow} . For complex mixtures, the HPLC method is ideal for determination of K_{ow} , and a range of values should be presented, with an indication of the proportion of substance within a given range (e.g. > 90 % of components have $\log K_{ow} > 6$), to allow the significance of these results to be reflected in the risk assessment. The HPLC method is also recommended for petroleum products, which are typically mixtures.

R.7.1.8.6 Endpoint specific information in the registration dossier / in IUCLID

Materials and methods

Shake-flask method (EU A.8/OECD TG 107):

- equilibrium concentrations of the test substance in both phases;
- relative volumes of the two phases;

- 1 • analytical method(s).
- 2 **Calculation method (EU A.8):**
- 3 • identification of the method;
- 4 • working principle of the method;
- 5 • reference to the method;
- 6 • identification of the data base;
- 7 • detailed information on the choice of fragments;
- 8 • applicability of the method.
- 9 **HPLC method (EU A.8/OECD TG 117):**
- 10 • column(s) used;
- 11 • mobile phase (composition, buffer, pH);
- 12 • reference substances with respective Kow values from the literature;
- 13 • concentrations measured.
- 14 **pH metric method (OECD TG 122):**
- 15 • description of the equipment;
- 16 • method and pH range of calibration of the electrode and standardisation of titrants;
- 17 • temperature of determinations;
- 18 • ionic strength of aquatic solution, and substance(s) used for maintaining the desired ionic strength;
- 19 • mass of the sample used, volume of ionic-strength adjusted water and volume of octanol;
- 20 • typical titration curve(s), pKa in aqueous solution and how it was obtained.
- 21 **slow-stirring method (OECD TG 123):**
- 22 • label purity of labelled substances and molar activity (where appropriate);
- 23 • sampling times;
- 24 • description of the test vessels and stirring conditions;
- 25 • number of replicates;
- 26 • temperature during the experiment;
- 27 • volumes of 1-octanol and water at the beginning, during and remaining after the test;
- 28 • determined concentrations of the test substance in 1-octanol and water as a function of time;
- 29 • description of the test vessels and stirring conditions (geometry of the stirring bar and of the test
- 30 vessel, vortex height in mm, and when available: stirring rate) used;
- 31 • analytical methods used to determine the test substance (its repeatability and sensitivity) and the
- 32 method limit of quantification;
- 33 • sampling times;
- 34 • pH of the aqueous phase and of the buffers used, when pH is adjusted for ionisable molecules;
- 35 • number of replicates;
- 36 • demonstration of mass balance;
- 37 • temperature and standard deviation or the range of temperature during the experiment;
- 38 • the regression of concentration ratio against time.
- 39 **Results and discussion**
- 40 • final value for log Kow;
- 41 • Kow values and their mean;
- 42 • standard deviations of individual Kow values;
- 43 • theoretical value when it has been calculated;
- 44 • temperature of the test solutions (°C);
- 45 • pH value(s) of the aqueous solution(s);
- 46 • composition and concentration of buffers;
- 47 • concentration of the stock solution.
- 48 If there are any deviations from the guideline method used or other special considerations then these
- 49 should be reported. In cases where there is more than one source of data, the endpoint summary
- 50 under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on partition coefficient can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.7	VII 7.8	Partition coefficient	E.4.8	3.6

R.7.1.8.7 References on *n*-octanol/water partition coefficient

Abraham M.H., Chadha H.S. and Mitchell R.C. Hydrogen bonding. 32. An analysis of water-octanol and water-cyclohexane partitioning and the log P parameter of Seiler. *J. Pharm. Sci.*(1994) 83, 1085-1100.

Bodor N, Gabanyi N.Z. and Wong C.-K. A new method for the estimation of partition coefficient. *J. Am. Chem. Soc.* (1989) 111, 3783-3786.

CEC (1993). Directive 67/548/EEC; Annex V Test Methods: A8: Partition Coefficient.

Dearden JC. Molecular structure and drug transport. In Ramsden CA (Ed.), *Comprehensive Medicinal Chemistry*, vol. 4, Pergamon Press, Oxford, 1990, pp. 375-411.

Dearden J.C., Netzeva T.I., Bibby R. A comparison of commercially available software for the prediction of partition coefficient, in Ford M., Livingstone D., Dearden J. and van de Waterbeemd H. (Eds.), *Designing Drugs and Crop Protectants: Processes, Problems and Solutions*, Blackwell, Oxford, 2003, pp. 168-169.

Dearden JC, Bresnen GM (2005). Thermodynamics of water-octanol and water-cyclohexane partitioning of some aromatic compounds. *Int. J. Mol. Sci.* 6, 119-129.

ECETOC (2003). QSARs: Evaluation of the commercially available software for human health and environmental endpoints with respect to chemical management applications. Technical Report 89. ECETOC, Brussels.

Ghose A.K., Pritchett A. and Crippen G.M. Atomic physico-chemical parameters for three dimensional structure directed quantitative structure-activity relationships: III. Modelling hydrophobic interactions. *J. Comput. Chem.* (1988) 9, 80-90.

GHS (2003). Globally Harmonised System of Classification and Labelling of Chemicals (GHS). United Nations, New York & Geneva.

Kapoor, I.; Metcalf, R.; Hirwe, A.S.; Coats, J.R.; Khalsa, M.S.; "Structure activity correlations of biodegradability of DDT analogs" *J. Agr. Food Chem.* (1973) 21, 310-315.

Klopman G. and Wang S. A computer automated structure evaluation (CASE) approach to calculation of partition coefficient. *J. Comput. Chem.* (1991) 12, 1025-1032.

Klopman G. and Zhu H. Recent methodologies for the estimation of *n*-octanol/water partition coefficients and their use in the prediction of membrane transport properties of drugs. *Mini-Rev. Med Chem.* (2005) 5, 127-133.

- 1 Leo A. Octanol/water partition coefficients. In Boethling R.S. and Mackay D. (Eds.), *Handbook of*
2 *Property Estimation Methods for Chemicals*. Lewis, Boca Raton, FL, 2000, pp. 89-114.
- 3 Livingstone D.J. Theoretical property predictions. *Current Topics in Med. Chem.* (2003) **3**, 1171-
4 1192.
- 5 Lyman W.J. Octanol/water partition coefficient. In Lyman W.J., Reehl W.F. and Rosenblatt D.H.
6 (Eds.), *Handbook of Chemical Property Estimation Methods*. American Chemical Society,
7 Washington DC, 1990, pp. 1.1-1.54.
- 8 Nendza M. *Structure-Activity Relationships in Environmental Sciences*. Chapman & Hall, London,
9 1998.
- 10 OECD (1989). OECD Guideline for the Testing of Chemicals: 117, Partition Coefficients. By
11 Reverse Phase Chromatography. OECD, Paris.
- 12 OECD (1995) OECD Guideline for the Testing of Chemicals: 107, Partition Coefficients. OECD,
13 Paris.
- 14 OECD (2000). LogK_{ow} pH-metric Method for Ionisable Substances. Organisation for Economic
15 Cooperation and Development (OECD), OECD Guideline for the Testing of Chemicals, Proposal
16 for a new Test Guideline 122 (draft November 2000), Paris.
- 17 OECD (2003) . OECD Draft Guideline for the Testing of Chemicals: 125, Partition Coefficients.
18 Slow-stirring method. OECD, Paris.
- 19 Reinhard M. and Drefahl A. Estimating Physico-chemical Properties of Organic Compounds.
20 Wiley, New York, 1999.
- 21 Schwarzenbach R.P., Gschwend P.M. and Imboden D.M. Environmental Organic Chemistry.
22 Wiley, New York, 1993.
- 23 Yalkowsky SH, Valvani SC, Roseman TJ. (1983) Solubility and partitioning. 6. Octanol solubility
24 and octanol-water partition coefficients. *J. Pharm. Sci.* 72, 866-870.

R.7.1.9 FLASH POINT

R.7.1.9.1 Type of property

The flash point is a property:

- for substance characterization;
- for the classification of flammable liquids.

R.7.1.9.2 Definition

The flash point is the lowest temperature of the liquid (as measured in a prescribed manner) at a pressure corrected to 101.3 kPa, at which application of an ignition source causes the vapour of the liquid to ignite momentarily and the flame to propagate across the surface of the liquid under the specified conditions of test.

R.7.1.9.3 Test method(s)

Suitable methods are listed in the CLP Regulation Annex I, 2.6.4.4, Table 2.6.3. Open cup methods are no longer allowed.

The method to be used has to be chosen taking into account the properties of the liquid (viscosity, halogenated compounds present) and the scope of the standard.

For substances with a high decomposition potential, a method using small amounts of liquid (e.g. EN ISO 3679: *Determination of flash point - Rapid equilibrium closed cup method*) is recommended to reduce the amount of substance under test.

For classification purposes it is recommended to use the mean of at least two test runs. If the experimentally determined flashpoint is found to be within ± 2 °C of the limiting criterion for classification or assigning a category when using a non-equilibrium method, it is recommended to repeat the determination with an equilibrium method.

R.7.1.9.4 Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

Column 2 of REACH Annex VII provides the following specific rules for adaptation of the standard information requirement for flash point:

The study does not need to be conducted if:

- *The substance is inorganic;*
- *The substance only contains volatile organic components with flash-points above 100 °C for aqueous solutions; or*
- *The estimated flash-point is above 200°C; or*
- *The flash-point can be accurately predicted by interpolation from existing characterised materials.*

The first bullet point has to be further specified as:

- The substance is inorganic except where there are covalent bonds;

1 Because some inorganic liquids with covalent bonds are flammable e.g. CS₂.
 2 The second bullet point should not be applied because it is unclear whether the 100 °C refers to the
 3 volatile organic components or to the aqueous solution. It is also not relevant in most cases anyway
 4 because it does not apply to pure substances.

5 The third bullet point should only be applied when a well validated estimation model was used.

6
 7 Waiving possibilities according to Annex XI to REACH

8 **Use of existing data: Data on physical-chemical properties from experiments not carried out**
 9 **according to GLP or the test methods referred to in Article 13 (3) of REACH**

10 The use of existing experimental data is possible if carried out with a closed cup method by
 11 certified institutions.

12 **Weight of evidence**

13 For the determination of the flash point, weight of evidence is not possible.

14 **(Q)SAR**

15 For the determination of the flash point, QSAR approaches are discouraged for the purpose of
 16 classification / risk assessment, except where the mean absolute error of the QSAR is less than
 17 2 °C.

18 For non-halogenated liquids calculation based on the vapour pressure curve and lower explosion
 19 limit of the substance can be used as a screening test and a flashpoint need not be determined
 20 experimentally if the calculated value is at least 5 °C higher than the relevant classification
 21 criterion.

22 **Grouping of substances and read-across approach**

23 At present grouping and read across are not applicable. Interpolation within homologous series may
 24 however be possible.

25 **Testing is technically not possible**

26 This applies if:

- 27 • the liquid is an explosive;
- 28 • the liquid is pyrophoric or self-reactive;
- 29 • decomposition occurs during the melting point study.

30 Further waiving possibilities

31 The flash point does not need to be determined experimentally if conclusive and consistent
 32 literature data are available.

33 Data generated with the same tests and classification principles as specified in the CLP Regulation
 34 for viscosity generated in conjunction with transport classification can satisfy the REACH
 35 requirements on a case-by-case basis.

R.7.1.9.5 Impurities; uncertainties

Impurities can have a significant influence on the flash point. The influence depends on the amount and the vapour pressure of the impurity. Even if their concentration is below 0.5 %, especially if their boiling point is substantially lower, they may have a strong effect on the flash point. Impurities with a higher boiling point will normally have no effect on the flashpoint.

R.7.1.9.2 Endpoint specific information in the registration dossier / in IUCLID**Materials and methods**

- reference to the standard or the test method applied;
- open cup or closed cup (for classification purposes only the closed cup methods are allowed);
- equilibrium or non-equilibrium method;
- type of ignition source;
- number of repetitions.

Results and discussion

- corrected flashpoint and unit;
- data on repeatability and reproducibility as given in the method.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on flash point can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.11	VII 7.9	Flash point	E.4.12	3.9

R.7.1.10 FLAMMABILITY

Some of the information requirements according to REACH Annex VII were phrased in a way that they correspond to ‘indications of danger’ as given in Annex II of the DSD. For substances, classification and labelling according to CLP Regulation has been mandatory since 1st December 2010 (and will become mandatory for mixtures (preparations) from 1st June 2015, when the DSD will be repealed). Consequently properties associated with flammability are covered by classification of the substance according to the CLP Regulation. However, the physical hazards according to the CLP Regulation are structured completely differently from the physico-chemical properties according to the DSD (and therefore also REACH, Annex VII). This means that for some of the CLP hazard classes an unambiguous assignment to one of the headlines (information requirements) in Annex VII to REACH is not possible. The assignment of hazard classes to the headline ‘Flammability’ as shown in the table below must therefore only be understood as a means to structure this document in accordance with Annex VII to REACH. It has to be noted that self-reactive substances and organic peroxides are assigned to the headline ‘Explosive properties’ as well because they can have explosive and/or flammable properties.

Table x Assignment of CLP hazard classes to the information requirement ‘Flammability’ according to REACH, Annex VII and correlation between the Test Method Regulation and the test method according to CLP and supporting link with the Guidance on the Application of the CLP Criteria.

REACH 1907/2006 (the no. in brackets is the respective no. in the table of REACH Annex VII)	Related hazard class according to CLP Regulation 1272/2008 (the no. in brackets is the respective chapter no. in Annex I to CLP)	Chapter in revised R.7(a) guidance	Test method according to the Test Method Regulation 440/2008	Test method according to the CLP Regulation	Chapter in the Guidance on the Application of the CLP Criteria (ex RIP 3.6)
7.10 Flammability	Flammable gases (2.2)	7.1.10.1	A.11	ISO 10156 EN 1839	2.3
	Flammable aerosols (2.3)	7.1.10.2	/	UN Section 31	2.4
	Flammable liquids (2.6)	7.1.10.3	see Flash point and Boiling point	see Flash point and Boiling point	2.7
	Flammable solids (2.7)	7.1.10.4	A.10	UN Test N.1	2.8
	Self-reactive substances and mixtures (2.8)	7.1.10.5	/	UN Test series A to H	2.9
	Pyrophoric liquids (2.9)	7.1.10.6	A.13	UN Test N.3	2.10
	Pyrophoric solids (2.10)	7.1.10.7	A.13	UN Test N.2	2.10
	Self-heating substances and mixtures (2.11)	7.1.10.8 (and 7.1.11.2)	/	UN Test N.4	2.11

	Substances and mixtures which in contact with water emit flammable gases (2.12)	7.1.10.9	Substances and mixtures which in contact with water emit flammable gases (2.12)	UN Test N.5	2.12
	Organic peroxides (2.15)	/	Organic peroxides (2.15)	UN Test series A to H	2.14

1

2 In addition, it has to be noted that some substances have flammable properties which do not result
3 in classification. Examples are the following:

- 4 • Gases that do not have a flammable range at 20 °C and standard pressure (and therefore are
5 not classified as flammable gases) might have a flammable range at higher temperatures
6 and/or pressure (e.g. refrigerant R134a);
- 7 • Liquids that do not have a flash point (and therefore are not classified as flammable liquids)
8 might have an explosion range (especially halogenated hydrocarbons).

9

10 Information about such properties should also be indicated in the dossier.

11 **R.7.1.10.1 Flammable gases**

12 Definition

13 Flammable gas means a gas or gas mixture having a flammable range with air at 20 °C and a
14 standard pressure of 101.3 kPa (Annex I to CLP, Section 2.2.1).

15 Classification criteria and relevant information

16 Flammable gases are classified into two categories depending on their flammability range: Flam.
17 Gas 1, H220; Flam. Gas 2, H221 (Annex I to CLP, Section 2.2.2. Table 2.2.1).

18 Detailed guidance on the classification criteria and the test method(s) can be found in the *Guidance*
19 *on the application of the CLP Criteria*, section 2.3.

20 Adaptation of the standard testing regime

21 **Waiving possibilities according to column 2 of Annex VII to REACH**

22 Column 2 of REACH Annex VII provides the following specific rules for adaptation of the standard
23 information requirement for flammability:

24 *The study does not need to be conducted:*

- 25 – *if the substance is a solid which possesses explosive or pyrophoric properties. These properties*
26 *should always be considered before considering flammability; or*
- 27 – *for gases, if the concentration of the flammable gas in a mixture with inert gases is so low that,*
28 *when mixed with air, the concentration is all time below the lower limit; or*
- 29 – *for substances which spontaneously ignite when in contact with air.*

30 The relevant bullet points can be paraphrased, namely the study does not need to be conducted:

- if the gas is known to be non-flammable;
- if the gas spontaneously ignites when in contact with air.

Examples of the gases known not to be flammable are argon, carbon dioxide, helium, krypton, nitrogen, xenon.

Gases that spontaneously ignite in contact with air are pyrophoric and therefore are flammable gases.

Waiving possibilities according to Annex XI to REACH

USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS REFERRED TO IN ARTICLE 13 (3) OF REACH

Many gases are classified in Annex VI to CLP either as *Flam. Gas 1* or *Flam. Gas 2*, and additional flammable gases are listed in the UN – RTDG whose classifications correspond to *Flam. Gas 1* according to CLP.

WEIGHT OF EVIDENCE

For gases that are not classified in Annex VI to the CLP Regulation nor in the UN-RTDG, there is ample scientific literature giving the flammability range for most gases (e.g. IEC 60079-20-1 “*Data for flammable gases and vapours, relating to the use of electrical apparatus*” – (under revision) or the databank Chemsafe at www.dechema.de/en/chemsafe.html).

(Q)SAR

At present (Q)SAR is generally not applicable for determination of explosion (/flammability) limits of gases.

GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH

At present grouping and read across are not applicable.

TESTING IS TECHNICALLY NOT POSSIBLE

In this case testing should always be possible.

Further waiving possibilities

Not foreseen.

Impurities; uncertainties

Tests should be performed with the lowest concentration of impurities in the gas encountered in the normal manufacturing process and the moisture content should be less than or equal to 0.01 %.

How to conclude on the DSD classification

All gases with a flammability range in air are classified ‘Extremely flammable F+ ; R12’ according to DSD, unless classified differently according to Annex VI, Table 3.2 of CLP Regulation. This

means that all gases classified as flammable gases according to CLP (either category 1 or 2) are classified as ‘Extremely flammable F+; R12’.

Endpoint specific information in the registration dossier/in IUCLID

Material and methods:

- description of the apparatus and dimensions or reference to the standard or the test method applied;
- test temperature;
- tested concentrations.

Results and discussion & Applicant’s Summary and conclusion (interpretation of results)

- indicate lower and upper explosion limits.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on flammability can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.13	VII 7.10	Flammability	E.4.14	3.11

Further information / references

For the testing of flammable gases according to CLP classification requirements, refer also to the *Guidance on the Application of the CLP Criteria*, section 2.3.

R.7.1.10.2 Flammable aerosols

The category of the flammable aerosols does not fall under the REACH registration requirements (Article 14 (4) REACH). Detailed guidance on the classification criteria and the test method(s) can be found in the *Guidance on the application of the CLP Criteria*, section 2.4.

R.7.1.10.3 Flammable liquids

Definition

Flammable liquid means a liquid which may form flammable/explosive vapour-air mixtures. Within the CLP Regulation ‘Flammable liquid’ means a liquid having a flashpoint of not more than 60 °C (see CLP Annex I, section 2.6.4.3).

Classification criteria and relevant information

Flammable liquids are classified in three categories according to the criteria of the CLP Regulation (see section 2.11, table 2.11.1) based on their boiling point and their flash point. Derogation is possible (CLP Annex I, section 2.6.4.5) for Flam. Liquid Cat. 3 having a flashpoint above 35 °C based on the information on sustained combustibility.

In addition EUH018 - 'In use, may form flammable/explosive vapour-air mixture' has to be assigned to substances classified under the CLP Regulation which may form flammable/explosive vapour-air mixtures although they do not have a flash point e. g. CH_2Cl_2 , $\text{C}_2\text{H}_3\text{Cl}_3$. In such cases it is possible to make the decision on whether flammable/explosive vapour-air mixture may be formed based on either the determination of explosion limits according to EN 1839 or the determination of explosion points according to EN 15794. It is sufficient to determine either the lower explosion limit or the lower explosion point.

Detailed guidance on the classification criteria and the test method(s) can be found in the *Guidance on the application of the CLP Criteria*, section 2.7.

Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

The entries 'flammability' (7.10), 'boiling point' (7.3) and 'flashpoint' (7.9) are the relevant ones.

Flammability:

Annex VII to REACH does not require to conduct testing for substances which spontaneously ignite when in contact with air.

Boiling point:

Annex VII to REACH does not require determination of the boiling point for substances which decompose before boiling (e.g. auto-oxidation, rearrangement, degradation, decomposition, etc.).

Flashpoint:

Annex VII to REACH does not require determination of the flash point if:

- *the substance is inorganic; or*
- *the substance only contains volatile organic components with flash-points above 100°C for aqueous solutions; or*
- *the estimated flash-point is above 200°C; or*
- *the flash-point can be accurately predicted by interpolation from existing characterised materials.*

The second bullet point should not be applied because it is unclear whether the 100 °C are referring to the volatile organic components or to the aqueous solution. It is also not relevant in most cases anyway because it does not apply to pure substances.

Waiving possibilities according to Annex XI to REACH

USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS REFERRED TO IN ARTICLE 13 (3) OF REACH

The use of existing data is possible if carried out using a closed cup method by qualified institutions.

WEIGHT OF EVIDENCE

For the determination of the flammable liquids, weight of evidence is not possible.

(Q)SAR

Boiling point:

Only some calculation methods based on increments give satisfying results. With respect to the relevant figure for flammable liquids (35 °C) only such methods with a mean absolute error lower than 2 °C in the range of 35 °C could be recommended.

Flash point:

(Q)SAR approaches are discouraged for the purposes of classification / risk assessment, except when their mean absolute error is lower than 2 °C.

For non-halogenated liquids calculation based on the vapour pressure curve and lower explosion limit of the substance can be used as a screening test and a flashpoint need not be determined experimentally if the calculated value is at least 5 °C higher than the relevant classification criterion. However in any case care has to be taken because of the influence of impurities on flashpoint (see below chapter on Impurities; uncertainties). For further reference see also the *Guidance on the Application of the CLP Criteria*, section 2.7.

Sustained Combustibility:

No (Q)SAR exists currently.

GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH

Boiling point:

At present grouping and read-across are not applicable. Interpolation within homologous series may however be possible.

Flash point:

At present grouping and read-across are not applicable.

Sustained Combustibility:

At present grouping and read-across are not applicable.

TESTING IS TECHNICALLY NOT POSSIBLE

Testing is not possible if:

- the liquid is an explosive;
- the liquid is pyrophoric or self-reactive.

Further waiving possibilities

Use of data on boiling point, flashpoint when determined with a closed cup method, explosion limits or lower explosion point from validated literature (see below chapter Further information/ references) is possible.

Data on boiling point generated in relation to transport classification may also satisfy the Annex XI requirements.

Data on flashpoint generated in relation to with transport classification may satisfy the Annex XI requirements if closed cup methods have been used. However care has to be taken in cases where there is no transport classification as “flammable liquid”, because certain substances can form flammable/explosive vapour-air mixtures although they do not have a flash point.

Impurities; uncertainties

Boiling point:

Impurities will influence the boiling point of the main component. The influence depends on the amount and boiling point of the impurity. The higher the amount and the higher the difference between the boiling points of the main component and the impurity, the higher the influence.

Flashpoint:

Special care has to be taken when a sample contains impurities with a lower boiling point than the main component. Even if their concentration is below 0.5 %, especially if their boiling point is substantially lower, they may have a strong effect on the test result. Impurities with a higher boiling point will normally have no effect on the flashpoint.

Sustained combustibility:

Impurities with lower boiling point may influence the ability to sustain combustion. However it is not yet possible to quantify the influence of impurities.

How to conclude on the DSD classification

Based on the data on boiling point and flashpoint the DSD classification according to the respective DSD criteria is possible. Simplified direct translation between CLP classification and DSD classification is not possible, see figure below.

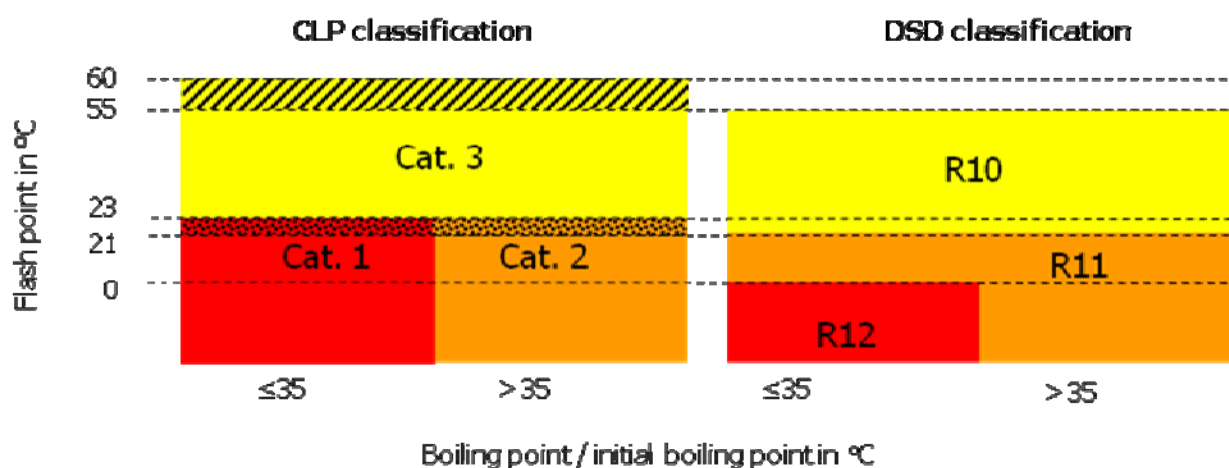


Figure xx: Comparison of the DSD and the CLP classification

Substances exempted from classification in Cat. 3 because of their flashpoint and behaviour when tested for sustained combustibility can also be exempted from being classified under DSD as R10 if they don't show additional dangerous properties relevant for classification.

No corresponding DSD classification exists for substances which have to be marked as EU H018 under CLP.

Endpoint specific information in the registration dossier/in IUCLID

Material and methods

See chapter flash point R.7.1.9 and boiling point R.7.1.3.

Results and discussion

- corrected flashpoint and unit;
- data on repeatability and reproducibility as given in the method;
- boiling point value (°C) as measured;
- pressure value and unit;
- rate of temperature increase;
- decomposition (if applicable);
- uncertainty in measurements;
- boiling point value in °C (corrected to standard pressure, except where the boiling point was determined at reduced pressures) (as above, but in a separate block of fields);
- if available explosion limits.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on flammability can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.13	VII 7.10	Flammability	E.4.14	3.11

Further information / references

See also R.7.1.3 Boiling point and R.7.1.9 Flash point. For testing of flammable liquids according to CLP classification requirements refer also to the *Guidance on the Application of the CLP Criteria*, section 2.7.

R.7.1.10.4 Flammable solids

Definition

A flammable solid means a solid which is readily combustible, or may cause or contribute to fire through friction. Readily combustible solids are powdered, granular, or pasty substances or mixtures which are dangerous if they can be easily ignited by brief contact with an ignition source, such as a burning match, and if the flame spreads rapidly.

1 Classification criteria and relevant information

2 Solid substances and mixtures are classified as flammable in two categories according to their
3 burning behaviour (see the CLP Regulation, Annex I, section 2.7) using method N.1 as described in
4 section 33.2.1 of the UN Recommendations on the Transport of Dangerous Goods, Manual of Tests
5 and Criteria.

6 Chapter 2.8 of the *Guidance on the Application of the CLP Criteria* gives detailed information on
7 the CLP classification of flammable solids, the N.1-test method and the relation to the DSD and the
8 Transport of Dangerous Goods regulations.

9 Adaptation of the standard testing regime

10 **Waiving possibilities according to column 2 of Annex VII to REACH**

11 Column 2 of REACH Annex VII provides the following specific rules for adaptation of the standard
12 information requirement for flammable solids.

13 *The study does not need to be conducted:*

- 14 – *if the substance is a solid which possesses explosive or pyrophoric properties. These properties*
15 *should always be considered before considering flammability; or*
16 – *for substances which spontaneously ignite when in contact with air.*

17 Testing for flammability of a solid is a part of classification in CLP Regulation. Refer also to the
18 *Guidance on the Application of the CLP Criteria*, section 2.8 on classification requirements.

19 For substances having explosive properties, testing for a classification as a flammable solid may be
20 waived. This applies to substances and mixtures classified as explosives, organic peroxides and
21 self-reactive substances and mixtures.

22 Substances which spontaneously ignite when in contact with air are pyrophoric substances as
23 defined by the CLP Regulation (see the *Guidance on the Application of the CLP Criteria*, section
24 2.10). Such substances are not classified as flammable solids but as pyrophoric solids under the
25 CLP Regulation.

26 **Waiving possibilities according to Annex XI to REACH**

27 **USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM**
28 **EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS**
29 **REFERRED TO IN ARTICLE 13 (3) OF REACH**

30 Literature data – even if available – should not be used since flammability strongly depends on
31 particle size, surface treatment and other parameters.

32 The use of existing data is possible provided that the test has been carried out by a certified
33 institution. If available data from an A.10 test indicate that a classification as a flammable solid
34 does not apply (result: not highly flammable), no more testing is necessary. However, if the A.10
35 test has come to the conclusion ‘highly flammable’, it will be necessary to also determine the
36 influence of the wetted zone as described in the UN N.1 test.

WEIGHT OF EVIDENCE

For inorganic materials, testing may be waived in cases where the substance is commonly known to be not flammable (i.e. stable salts or metal oxides) or where a flammability hazard can be excluded by any other scientific reasoning.

(Q)SAR

At present (Q)SAR is generally not applicable for flammable solids. Application of (Q)SAR is not possible.

GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH

At present, grouping and read across are not applicable.

TESTING IS TECHNICALLY NOT POSSIBLE

In this case, testing should always be possible.

Further waiving possibilities

If a suitable screening test clearly shows that the substance is not flammable, further testing is not necessary (see also the *Guidance on the application of the CLP Criteria*, section 2.8.4.2). An example for a suitable screening test is the burning index as described in VDI guideline (VDI Guideline, 1990) if a burning index of 3 or less is found, the substance should not be classified as a flammable solid and no further testing is required.

Substances and mixtures classified according to the CLP Regulation as explosives, organic peroxides, self-reactive substances and mixtures as well as pyrophoric or oxidising solids should not be considered for classification as flammable solids since flammability is an intrinsic hazard in these classes (see the *Guidance on the Application of the CLP criteria*, section 2.8.3).

However, if a substance gives a positive result in Test Series 1 or 2 as described in the UN Manual of Tests and Criteria, but is exempted from classification as an explosive on the basis of Test Series 6, a test for classification as a flammable solid should be performed.

Impurities; uncertainties

Impurities do not tend to have a large effect on the flammability of a solid. However, if a solid which is not flammable in the pure state contains flammable organic liquids or organometallic impurities it may burn more rapidly and thus become flammable.

How to conclude on the DSD classification

Any substance found to be a flammable solid according to CLP Regulation has to be classified as 'F; R11' according to the DSD.

Endpoint specific information in the registration dossier/in IUCLID

Material and methods

- description of the apparatus and dimensions or reference to the standard or the test method applied;

Solid flammability:

- indicate if preliminary and/or main test performed;
- moisture content;
- Particle size and distribution (if available).

Results and discussion

- indicate burning time;
- pass/non pass of the wetted zone (in the case of the N.1 method).

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on flammability can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.13	VII 7.10	Flammability	E.4.14	3.11

Further information / references

VDI guideline 2263, part 1, (1990): “Test methods for the Determination of the Safety Characteristics of Dusts”.

R.7.1.10.5 Self-reactive substances and mixtures**Definition**

The definition of a self-reactive substance is given in CLP Regulation Annex I, section 2.8.1.

Self-reactive substances or mixtures are thermally unstable liquid or solid substances or mixtures liable to undergo a strongly exothermic decomposition even without participation of oxygen (air). This definition excludes substances and mixtures classified according to this Part as explosives, organic peroxides or as oxidising.

A self-reactive substance or mixture is regarded as possessing explosive properties when in laboratory testing the formulation is liable to detonate, to deflagrate rapidly or to show a violent effect when heated under confinement.

Background information and guidance on the definition is given in the *Guidance on the Application of the CLP Criteria*, sections 2.9.1 and 2.9.2.

Classification criteria and relevant information

Classification principles are given in CLP Regulation Annex I, sections 2.8.2 and 2.8.4.

Background information and guidance on relevant aspects regarding the classification is given in the *Guidance on the Application of the CLP Criteria*, sections 2.9.3, 2.9.5 and 2.9.6.

Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

Only self-reactive substances, as defined in the section definition, have to be tested according to the United Nations Manual of Tests and Criteria, Part II test series A - H.

CLP Annex I provides the following specific rules for adaptation of the standard information requirement for self-reactive substances and mixtures.

Any self-reactive substance or mixture shall be considered for classification in this class as a self-reactive substance or mixture unless:

(a) they are explosives, according to the criteria given in 2.1;

(b) they are oxidising liquids or solids, according to the criteria given in 2.13 or 2.14, except that mixtures of oxidising substances, which contain 5 % or more of combustible organic substances shall be classified as self-reactive substances according to the procedure defined in 2.8.2.2;

(c) they are organic peroxides, according to the criteria given in 2.15;

(d) their heat of decomposition is less than 300 J/g; or

(e) their self-accelerating decomposition temperature (SADT) is greater than 75 °C for a 50 kg package

(See UN Recommendations on the Transport of Dangerous Goods, Manual of Tests and Criteria, sub-sections 28.1, 28.2, 28.3 and Table 28.3.)

Waiving possibilities according to Annex XI to REACH

USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS REFERRED TO IN ARTICLE 13 (3) OF REACH

A number of already tested and classified substances and mixtures are listed in United Nations Recommendations on the Transport of Dangerous Goods, section 2.4.2.3.2.3. Available information may originate from the classification for transport. More details are given in the *Guidance on the Application of the CLP Criteria*, sections 1.7.2.1 and 2.9.5.

WEIGHT OF EVIDENCE

For the determination of the self-reactive substances and mixtures, weight of evidence is not possible.

(Q)SAR

At present (Q)SAR is generally not applicable for determination of self-reactive substances. Application of (Q)SAR is not possible.

GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH

At present grouping and read-across are not applicable.

1 **TESTING IS TECHNICALLY NOT POSSIBLE**

2 A few of substances can, for safety reasons, only be handled and tested in diluted form, see the
3 substances and mixtures listed in UN TDG, section 2.4.2.3.2.3.

4 **Further waiving possibilities**

5 Not foreseen.

6 Impurities; uncertainties

7 Minor impurities can have an influence on thermal stability. Background information and guidance
8 on these aspects is given in the *Guidance on the Application of the CLP Criteria*, section 2.9.3.3.

9 How to conclude on the DSD classification

10 In the DSD self-reactive substances are not covered. They may be classified in other DSD classes
11 (e.g. explosive substance, flammable solid or liquid). However, in the CLP Regulation self-reactive
12 substances are classified as Type A (explosive), Type B (self-reactive substance and explosive) and
13 Types C-G (self-reactive substance). See also the *Guidance on the Application of the CLP Criteria*,
14 section 2.9.5.

15 What information is required in the registration dossier in IUCLID

16 **Material and methods**

17
18 See UN MTC, Part II, classification procedures and test series A-H.

20 **Results and discussion**

21
22 The following data on self-reactive substances should be submitted:

- 23
24 • type of self-reactive substance;
- 25 • decomposition energy (value and method of determination);
- 26 • SADT (Self accelerating decomposition temperature);
- 27 • detonation properties (Yes/Partial/No);
- 28 • deflagration properties (Yes rapidly/Yes slowly/No);
- 29 • effect of heating under confinement (Violent/Medium/Low/No);
- 30 • explosive power if applicable (Not low/Low/None).

31 For assigning the type of self-reactive substance, the list of currently assigned self-reactive
32 substances according to the 2.4.2.3.2.3 of the UN RTDG can be used, in cases where the assignment
33 was based on test(s) according to the UN Manual of Tests and Criteria. The relevant underlying test
34 data may be collected from the respective UN documents from the UN committee of experts on the
35 transport of dangerous goods, from test reports produced by competent authorities or industry, or
36 from other reliable sources.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on flammability can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.13	VII 7.10	Flammability	E.4.14	3.11

Further information / references

Background information and guidance on classification testing, additional testing and available information is given in the *Guidance on the Application of the CLP Criteria*, section 2.9.

R.7.1.10.6 Pyrophoric liquids

Definition

The definition of a pyrophoric liquid is given in the CLP Regulation Annex I, section 2.9.1.

Pyrophoric liquid means a liquid substance or mixture which, even in small quantities, is liable to ignite within five minutes after coming into contact with air.

Background information and guidance on the definition is given in the *Guidance on the Application of the CLP Criteria*, sections 2.10.1 and 2.10.2.

Classification criteria and relevant information

Classification principles are given in CLP Regulation Annex I, section 2.9.2.

The criterion for a pyrophoric liquid is as follows *The liquid ignites within 5 min when added to an inert carrier and exposed to air, or it ignites or chars a filter paper on contact with air within 5 min.*

Background information and guidance on relevant aspects regarding the classification is given in the *Guidance on the Application of the CLP Criteria*, sections 2.10.1, 2.10.2, 2.10.3 and 2.10.4.

Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

Other flammability tests do not have to be performed as well as the determination of the self-ignition temperature, if the substance is a pyrophoric substance. However, flammability in contact with water may be relevant.

The classification procedure for pyrophoric liquids need not be applied when experience in manufacture or handling shows that the substance or mixture does not ignite spontaneously on

1 coming into contact with air at normal temperatures (i.e. the substance is known to be stable at
2 room temperature for prolonged periods of time (days)).

3 **Waiving possibilities according to Annex XI to REACH**

4 **USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM** 5 **EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS** 6 **REFERRED TO IN ARTICLE 13 (3) OF REACH**

7 The N.3 method of the UN Manual of Tests and Criteria is also used for classification according to
8 the regulations on the transport of dangerous goods (ADR and RID). If the liquid in question has
9 been classified as belonging to Class 4.2, packing group I of the ADR/RID on the basis of N.3 test
10 results, it is a pyrophoric liquid according to CLP criteria. Packing group I of the ADR/RID directly
11 corresponds to Category 1 of the CLP.

12 According to the DSD, the A.13 method of Regulation (EC) 440/2008 is used for the assessment of
13 pyrophoric properties for liquids and liquids. This method is identical to the N.3 test method.

14 **WEIGHT OF EVIDENCE**

15 For the determination of the pyrophoric liquids, weight of evidence is not possible.

16 **(Q)SAR**

17 Application of (Q)SAR is not possible, however assessment of the chemical structure may be used
18 to exclude pyrophoric properties of a substance.

19 **GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH**

20 Assessment of the chemical structure may be used to anticipate pyrophoric properties of a
21 substance.

22 **TESTING IS TECHNICALLY NOT POSSIBLE**

23 Due to pyrophoric properties a number of other tests on physical-chemical, toxicological and eco-
24 toxicological endpoints cannot be conducted.

25 **Further waiving possibilities**

26 Not foreseen.

27 Impurities; uncertainties

28 More background information and guidance on this and other aspects is given in the *Guidance on*
29 *the Application of the CLP Criteria*, section 2.10.

30 How to conclude on the DSD classification

31 Because the test methods of DSD and CLP are identical for this endpoint there is no difference in
32 classification, see also the *Guidance on the Application of the CLP Criteria*, section 2.10.6.

Endpoint specific information in the registration dossier IUCLID

Material and methods

Description of the apparatus and dimensions or reference to the standard or the test method applied.
Note that in this case the experience in handling may be sufficient.

Results and discussion

- whether ignition occurs when poured or whether the filter paper is charred.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on flammability can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.13	VII 7.10	Flammability	E.4.14	3.11

Further information / references

Background information and guidance on classification testing, additional testing and available information is given in the *Guidance on the Application of the CLP Criteria*, section 2.10.

R.7.1.10.7 Pyrophoric solids

Definition

The definition of a pyrophoric solid is given in CLP Regulation Annex I, section 2.10.1.

Pyrophoric solid means a solid substance or mixture which, even in small quantities, is liable to ignite within five minutes after coming into contact with air.

Background information and guidance on the definition is given in the *Guidance on the Application of the CLP Criteria*, sections 2.10.1 and 2.10.2.

Classification criteria and relevant information

Classification principles are given in CLP Regulation Annex I, section 2.10.2.

The criterion for a pyrophoric solid is as follows: *The solid ignites within 5 minutes of coming into contact with air.*

Background information and guidance on relevant aspects regarding the classification is given in the *Guidance on the Application of the CLP Criteria*, sections 2.10.1, 2.10.2, 2.10.3 and 2.10.4.

1 Adaptation of the standard testing regime

2 **Waiving possibilities according to column 2 of Annex VII to REACH**

3 Other flammability tests do not have to be performed in addition to the determination of the self-
4 ignition temperature, if the substance is a pyrophoric substance. However, flammability in contact
5 with water may be relevant.

6 The classification procedure for pyrophoric solids need not be applied when experience in
7 manufacture or handling shows that the substance or mixture does not ignite spontaneously on
8 coming into contact with air at normal temperatures (i.e. the substance is known to be stable at
9 room temperature for prolonged periods of time (days)).

10 **Waiving possibilities according to Annex XI to REACH**

11 **USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM**
12 **EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS**
13 **REFERRED TO IN ARTICLE 13 (3) OF REACH**

14 The N.2 method of the UN Manual of Tests and Criteria is also used for classification according to
15 the regulations on the transport of dangerous goods (ADR and RID). If the solid in question has
16 been classified as belonging to Class 4.2, packing group I of the ADR/RID on the basis of N.2 test
17 results, it is a pyrophoric solid according to CLP Regulation criteria. Packing group I of the
18 ADR/RID directly corresponds to Category 1 of CLP.

19 According to the DSD, the A.13 method of Regulation (EC) 440/2008 is used for the assessment of
20 pyrophoric properties for solids and liquids. This method is identical to the N.2 test method.

21 **WEIGHT OF EVIDENCE**

22 For the determination of the pyrophoric solids, weight of evidence is not possible.

23 **(Q)SAR**

24 Application of (Q)SAR is not possible, however assessment of the chemical structure may be used
25 to exclude pyrophoric properties of a substance.

26 **GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH**

27 Assessment of the chemical structure may be used to anticipate pyrophoric properties of a
28 substance.

29 **TESTING IS TECHNICALLY NOT POSSIBLE**

30 Due to pyrophoric properties a number of other tests on physicochemical, toxicological and
31 ecotoxicological endpoints cannot be conducted.

32 **Further waiving possibilities**

33 Not foreseen.

Impurities; uncertainties

Particle size may play an important role. More background information and guidance on this and other aspects is given in the *Guidance on the Application of the CLP Criteria*, section 2.10.

How to conclude on the DSD classification

Because the test methods of DSD and CLP Regulation are identical for this endpoint there is no difference in classification, see also the *Guidance on the Application of the CLP Criteria*, section 2.10.6.

Endpoint specific information in the registration dossier/in IUCLID

Material and methods

- description of the apparatus and dimensions or reference to the standard or the test method applied;
 - particle size and distribution (if practicable);
- Note that in this case experience in handling may be sufficient.

Results and discussion

- whether ignition occurs when poured;

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on flammability can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.13	VII 7.10	Flammability	E.4.14	3.11

Further information / references

Background information and guidance on classification testing, additional testing and available information is given in the *Guidance on the Application of the CLP Criteria*, section 2.10.

R.7.1.10.8 Self-heating substances and mixtures

Definition

For solids and liquids absorbed onto a large surface, self-heating may occur by reaction with air with subsequent ignition. According to the CLP Regulation, Annex I, section 2.11.1.1.:

A self-heating substance or mixture is a liquid or solid substance or mixture, other than a pyrophoric liquid or solid, which, by reaction with air and without energy supply, is liable to self-

1 *heat; this substance or mixture differs from a pyrophoric liquid or solid in that it will ignite only*
2 *when in large amounts (kilograms) and after long periods of time (hours or days).*

3 Classification criteria and relevant information

4 Self-heating substances and mixtures are classified in two categories according to the criteria of the
5 CLP Regulation (see section 2.11, table 2.11.1). In general, self-heating occurs only for solids in
6 contact with air. The *Guidance on the Application of the CLP Criteria*, section 2.11 gives detailed
7 background information about this phenomenon.

8 Adaptation of the standard testing regime

9 **Waiving possibilities according to column 2 of Annex VII to REACH**

10 Column 2 of the REACH Annex VII provides the following specific rules for adaptation of the
11 standard information requirement for self-ignition temperature.

12 *The study does not need to be conducted:*

- 13 – *if the substance is explosive or ignites spontaneously with air at room temperature; or*
- 14 – *for solids, if the substance has a melting point < 160°C, or if preliminary results exclude self-*
15 *heating of the substance up to 400°C.*

16
17 The *Guidance on the Application of the CLP Criteria*, section 2.11 should be consulted for details
18 about waiving and screening criteria. For the purposes of REACH, no data are required for solids
19 classified as:

- 20 • pyrophoric; or
- 21 • explosive, unstable or division 1.1 to 1.6; or
- 22 • organic peroxide; or
- 23 • self-reactive substance.

24
25 Further, no data are required for substances with a melting point below 160 °C. This means also that
26 liquids do not have to be tested for this endpoint for the purposes of this regulation. Annex VII of
27 REACH also allows waiving “if preliminary results exclude self-heating of the substance up to
28 400°C.” This refers to Test Method Regulation 440/2008, method A.16. However, the criteria are
29 not very clear, and therefore it is recommended to instead refer to the CLP Regulation classification
30 criteria, if applicable, and to waive otherwise.

31 **Waiving possibilities according to Annex XI to REACH**

32 **USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM** 33 **EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS** 34 **REFERRED TO IN ARTICLE 13 (3) OF REACH**

35 Literature data – even if available – should not be used since self-heating strongly depends on
36 particle size, surface treatment and other parameters.

37 The use of existing data is possible provided that the test has been carried out by a qualified
38 institution. If available data from a test according to A.16 indicate that a classification as a self-
39 heating substance does not apply, no more testing is necessary. However, the interpretation of the
40 A.16 test in terms of the CLP criteria requires appropriate expert knowledge.

WEIGHT OF EVIDENCE

For the determination of the self-heating substances and mixtures, weight of evidence is not possible.

(Q)SAR

At present (Q)SAR is generally not applicable for self-heating substances and mixtures. Application of QSAR is not possible.

GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH

At present grouping and read-across are not applicable.

TESTING IS TECHNICALLY NOT POSSIBLE

In some cases, exothermic decomposition may occur when performing the test, and special care will be necessary with respect to performing the tests and interpreting the results; see the *Guidance on the Application of the CLP criteria*, section 2.11.4.4.3. In such cases, it may not be possible to determine these properties.

Further waiving possibilities

According to the UN Manual of Tests and Criteria, the classification procedure for self-heating substances or mixtures need not be applied if the results of a screening test can be adequately correlated with the classification test and an appropriate safety margin is applied. Examples of screening tests are:

- (a) The Grewer Oven test (VDI guideline, 1990) with an onset temperature 80 K above the reference temperature for a volume of 1 litre;
- (b) The Bulk Powder Screening Test (Gibson et al., 1985) with an onset temperature 60 K above the reference temperature for a volume of 1 litre.

Impurities; uncertainties

Particle size may play an important role. More background information and guidance on this and other aspects is given in the *Guidance on the Application of the CLP Criteria*, section 2.11.

How to conclude on the DSD classification

This hazard class is not defined in DSD, therefore translation is not possible.

Endpoint specific information in the registration dossier/in IUCLID

Material and methods

- description of the apparatus and dimensions or reference to the standard or the test method applied;
- indicate if preliminary and/or main test performed;
- moisture content;
- particle size and distribution (if available).

Results and discussion

- indicate temperature rise obtained for the individual tests and classification result;

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on flammability can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.13	VII 7.10	Flammability	E.4.14	3.11

Further information / references

ECHA guidance document *the Guidance on the Application of the CLP Criteria* gives in section 2.11 detailed information on the self-heating property, the CLP-classification, the relevant test method and the relation to the DSD and the transport of dangerous goods regulations.

VDI guideline 2263, part 1 (1990): “Test methods for the Determination of the Safety Characteristics of Dusts”.

Gibson, N. Harper, D.J. Rogers (1985): “Evaluation of the fire and explosion risks in drying powders”, *Plant Operations Progress*, 4 (3), 181-189.

R.7.1.10.9 Substances which in contact with water emit flammable gases**Definition**

The CLP Regulation, Annex I, section 2.12.1 provides the following definition:

Substances or mixtures which, in contact with water, emit flammable gases means solid or liquid substances or mixtures which, by interaction with water, are liable to become spontaneously flammable or to give off flammable gases in dangerous quantities.

Classification criteria and relevant information

Classification according to the CLP Regulation is required if the gas produced upon contact with water ignites spontaneously and/or if the reaction rate with which the flammable gas is produced is ≥ 1 l/kg·h.

If the gas produced ignites spontaneously, this does not necessarily imply that the gas produced is pyrophoric but this generally is the case if the heat of reaction is sufficient to result in ignition of the gas.

The test method for classification of substances and mixtures which in contact with water emit flammable gases is described in the UN Manual of Tests and Criteria (UN Test N.5, see Section 33.4). This method is referred to in Annex I, Part 2 of the CLP Regulation and it is strongly recommended to use this method and not to apply test method A.12 of the Test Methods Regulation

if new testing is carried out. UN Test N.5 foresees dividing into three categories depending on the violence and rate of the reaction whereas test method A.12 does not allow any further dividing of the substances. Furthermore, the results of both methods might differ slightly due to some differences in the testing procedure (for these differences see the *Guidance on the Application of the CLP Criteria*, Section 2.12.5). Therefore unnecessary testing can be avoided by applying only UN Test N.5 because it leads to more detailed information (and has in any case to be applied for other purposes such as classification and transport).

Data which is based on the classification according to DSD may be available. There are, however, differences between the methods UN Test N.5 and A.12 which should be considered. They are described in detail in the *Guidance on the Application of the CLP Criteria*, section 2.12.5.

Detailed guidance on the test method itself can be found in the *Guidance on the Application of the CLP Criteria*, section 2.12.3.4.1.

Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

Column 2 of REACH Annex VII provides the following specific rules for adaptation of the standard information requirement for flammability.

The study does not need to be conducted:

- if the substance is a solid which possesses explosive or pyrophoric properties. These properties should always be considered before considering flammability; or*
- for gases, if the concentration of the flammable gas in a mixture with inert gases is so low that, when mixed with air, the concentration is all time below the lower limit; or*
- for substances which spontaneously ignite when in contact with air.*

The first bullet point is valid with regard to explosive substances because they are not classified as substances which in contact with water emit flammable gases. In that case testing can be waived.

The other waiving possibilities are not applicable with regard to substances which in contact with water emit flammable gases:

The first bullet point is not correct with regard to pyrophoric substances because pyrophoric substances can be classified as substances which in contact with water emit flammable gases based on UN Test N.5 which is referred to by CLP. UN Test N.5 explicitly requires testing of pyrophoric substances under nitrogen (see UN Manual of Tests and Criteria, section 33.4.1.3.1).

For the same reasons, the last bullet point (waiving would be possible for substances which spontaneously ignite when in contact with air) is also not valid in this case.

The second bullet point is not applicable because gases do not fall under the hazard class of substances which in contact with water emit flammable gases.

1 **Waiving possibilities according to Annex XI to REACH**

2 **USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM** 3 **EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS** 4 **REFERRED TO IN ARTICLE 13 (3) OF REACH**

5 Existing data that were generated by certified institutions may be used.

6 **WEIGHT OF EVIDENCE**

7 Waiving of testing is possible based on the following:

- 8 • Molecular structure:
9 Substances that do not contain metals or semimetals (generally) do not fulfil the criteria for
10 classification in this hazard class.
- 11 • Experience in handling and use:
12 If the substance is known to be soluble in water to form a stable solution, or if it is clearly
13 known that it does not react with water, e.g. because it is manufactured or washed with water,
14 testing is not necessary.

15 **(Q)SAR**

16 There are currently no QSPR models for predicting whether a substance in contact with water emits
17 flammable gases and if so what the gas evolution rate is.

18 **GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH**

19 At present grouping and read-across are not applicable.

20 **TESTING IS TECHNICALLY NOT POSSIBLE**

21 Testing should always be possible if none of the waiving possibilities applies.

22 **Further waiving possibilities**

23 Classification in certain hazard classes do not foresee the assignment of further physical hazard
24 classes or at least normally do not match with classification in this hazard class:

- 25 • Substances that are classified as explosives, self-reactives or organic peroxides are not
26 classified in this hazard class (or any other physical hazard class). For explosives this is
27 considered through the first bullet point of the waiving possibilities according to REACH
28 Annex VII, column 2 (see above).
- 29 • Oxidizing substances are generally not considered for flammability and therefore are also not
30 classified in this hazard class (there may be some exceptions, however).

31 Impurities; uncertainties

32 The descriptions of the methods UN Test N.5 and A.12 are not very detailed and therefore allow for
33 technical variations such as with regard to the apparatus used or the procedure. In particular, the
34 testing protocol does not prescribe a specific method for measuring the gas evolution rate. An

interlaboratory comparison for this test method has shown that laboratories - based on the freedom the description of the test methods gives - apply different approaches when performing this test. Furthermore, the interlaboratory comparison showed that the test results vary in a rather wide range. It therefore has to be kept in mind that this test method has a non-negligible uncertainty with regard to trueness and precision.

Sea water may be a particular case of interest (in case of maritime transport).

How to conclude on the DSD classification

Substances which in contact with water emit flammable gases would be classified as ‘F; R15’ under DSD (the sum of categories 1 to 3 corresponds to ‘F; R15’).

Endpoint specific information in the registration dossier/in IUCLID

Material and methods

- description of the apparatus and dimensions or reference to the standard or the test method applied;
- particle size and distribution.

Results and discussion

- indicate whether full test was performed or whether it was terminated at a particular step/stage;
- substance identity of evolved gas;
- indicate whether the gas evolved ignites spontaneously;
- rate of gas evolution (unless the test has been terminated).

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on flammability is found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.13	VII 7.10	Flammability	E.4.14	3.11

Further information / references

Janès et al, “Towards the improvement of UN N.5 test method intended to the characterization of substances which in contact with water emit Flammable Gases”, submitted in revised form to Journal of Loss Prevention in the Process Industries.

R.7.1.10.10 Organic peroxides

Definition

The definition of an organic peroxide is given in CLP Annex I, section 2.15.1:

Organic peroxide means a liquid or solid organic substance which contains the bivalent -O-O- structure and as such is considered a derivative of hydrogen peroxide, where one or both of the hydrogen atoms have been replaced by organic radicals. The term organic peroxide includes organic peroxide mixtures (formulations) containing at least one organic peroxide. Organic peroxides are thermally unstable substances or mixtures, which can undergo exothermic self-accelerating decomposition. In addition, they can have one or more of the following properties:

- (i) Be liable to explosive decomposition;*
- (ii) Burn rapidly;*
- (iii) Be sensitive to impact or friction;*
- (iv) React dangerously with other substances.*

An organic peroxide is regarded as possessing explosive properties when in laboratory testing the mixture (formulation) is liable to detonate, to deflagrate rapidly or to show a violent effect when heated under confinement.

Background information and guidance on the definition is given in *Guidance on the Application of the CLP Criteria*, sections 2.14.1 and 2.14.2.

Classification criteria and relevant information

The Classification principles are given in CLP Annex I, sections 2.15.2 and 2.15.4.

Background information and guidance on relevant aspects regarding the classification is given in *Guidance on the Application of the CLP Criteria*, sections 2.14.3, 2.14.4, 2.14.6, 2.14.7 and 2.14.8.

Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

Only organic peroxides, as defined in CLP, Annex I, section 2.15.1 definition, have to be tested according to the United Nations Manual of Tests and Criteria, Part II test series A - H.

The study does not need to be conducted if:

- *the substance or mixture contains:*

- (a) not more than 1.0% available oxygen from the organic peroxides when containing not more than 1.0% hydrogen peroxide; or*
- (b) not more than 0.5% available oxygen from the organic peroxides when containing more than 1.0% but not more than 7.0% hydrogen peroxide.*

NOTE:

The available oxygen content (%) of an organic peroxide mixture is given by the formula:

$$16 \times \sum_i^n \left(\frac{n_i \times c_i}{m_i} \right)$$

where:

n_i = number of peroxygen groups per molecule of organic peroxide i ;

1 c_i = concentration (mass %) of organic peroxide i ;

2 m_i = molecular mass of organic peroxide i .

3 **Waiving possibilities according to Annex XI to REACH**

4 **USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM**
5 **EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS**
6 **REFERRED TO IN ARTICLE 13 (3) OF REACH**

7 A number of already tested and classified substances and mixtures are listed in the United Nations
8 Recommendations on the Transport of Dangerous Goods, 2.5.3.2.4.

9 Available information may especially originate from the classification for transport. In the DSD
10 organic peroxides were classified as oxidizing substances, by definition. More details are described
11 in the *Guidance on the Application of the CLP Criteria*, sections 1.7.2.1 and 2.14.6.

12 **WEIGHT OF EVIDENCE**

13 For the determination of the organic peroxides, weight of evidence is not possible.

14 **(Q)SAR**

15 At present QSAR is generally not applicable for organic peroxides. Application of (Q)SAR is not
16 possible.

17 **GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH**

18 At present grouping and read across are not applicable.

19 **TESTING IS TECHNICALLY NOT POSSIBLE**

20 A number of substances can, for safety reasons, only be handled and tested in diluted form, see the
21 substances and mixtures listed in UN TDG, 2.5.3.2.4.

22 **Further waiving possibilities**

23 Not foreseen.

24 Impurities; uncertainties

25 Minor impurities can have an influence on thermal stability. Background information and guidance
26 on these aspects is given in *Guidance on the Application of the CLP Criteria*, section 2.14.4.

27 How to conclude on the DSD classification

28 In the DSD organic peroxides are classified as oxidizing substances and a few of them as having
29 explosive properties. However, in CLP Regulation organic peroxides are classified as Type A
30 (explosive), Type B (organic peroxide and explosive) and Types C-G (organic peroxide). See also
31 *Guidance on the Application of the CLP Criteria*, section 2.14.6.

Endpoint specific information in the registration dossier/in IUCLID**Material and methods**

- See UN MTC, Part II, classification procedures and test series A-H.

Results and discussion

The following data on organic peroxides should be submitted:

- type of organic peroxide;
- SADT (Self accelerating decomposition temperature);
- detonation properties (Yes/Partial/No);
- deflagration properties (Yes rapidly/Yes slowly/No);
- effect of heating under confinement (Violent/Medium/Low/No);
- explosive power, if applicable (Not low/Low/None).

For assigning the Type of organic peroxide, the list of currently assigned organic peroxides according 2.5.3.2.4 of the UN RTDG can be used, in case the assignment was based on a test according to the UN MTC. The relevant underlying test data may be collected from the respective UN documents from the UN committee of experts on the transport of dangerous goods, from test reports produced by either competent authorities or industry, or from other reliable sources (such as e.g. the dedicated database 'DATATOP').

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on flammability can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.13	VII 7.10	Flammability	E.4.14	3.11

Further information / references

Background information and guidance on classification testing, additional testing and available information is given in *Guidance on the Application of the CLP Criteria*, section 2.14.

Data from the 'DATATOP' database can be obtained from the gatekeeper of this database TNO, Department Energetic Materials, Lange Kleiweg 137, 2288GJ, Rijswijk The Netherlands.

R.7.1.11 EXPLOSIVE PROPERTIES

Some of the information requirements according to the REACH Regulation, Annex VII were phrased such that they correspond to ‘indications of danger’ as given in Annex II of DSD. For substances, classification and labelling according to the CLP Regulation has been mandatory since December 1, 2010 (and will become mandatory for mixtures (preparations) from June 1, 2015, when the DSD will be repealed). Consequently, explosive properties are covered by classification of the substance according to the CLP Regulation. However, the physical hazards according to CLP are structured completely differently from the physico-chemical properties according to the DSD (and therefore also REACH, Annex VII). This means that for some of the CLP hazard classes an unambiguous assignment to one of the headlines (information requirements) in Annex VII to REACH is not possible. The assignment of hazard classes to the headline ‘Explosive properties’ as shown in Table below must therefore only be understood as a means to structure this document in accordance with Annex VII to REACH. It has to be noted that self-reactive substances and organic peroxides are assigned to the headline ‘Flammability’ as well because they can have explosive and/or flammable properties.

Table x Assignment of CLP hazard classes to the information requirement ‘Explosive properties’ according to REACH, Annex VII and correlation between the Test method Regulation and the test method according to CLP and supporting link with the Guidance on the Application of the CLP Criteria.

REACH (the no. in brackets is the respective no. in the table of REACH Annex VII to IX)	Related hazard class according to the CLP Regulation (the no. in brackets is the respective chapter no. in Annex I to CLP)	Chapter in revised R.7(a) guidance	Test method according to the Test Method Regulation 440/2008	Test method according to the CLP Regulation	Chapter in the Guidance on the Application of the CLP Criteria (ex RIP 3.6)
7.11 Explosive properties	Explosives	7.1.11.1	A.14	UN Test series 1 to 3 (further test series 4 to 6 are necessary for classification)	2.2
	Self-reactive substances and mixtures	7.1.11.2	/	UN Test series A to H	2.9
	Organic peroxides	7.1.11.3	/	UN Test series A to H	2.14

In addition, it has to be noted that some substances have explosive properties which do not result in classification. Examples are the following:

- Substances with a positive result in UN test series 1 or 2 but which are exempted from the classification as explosives based on their packaging in UN test series 6;
- Substances which are mechanically sensitive only. These are substances with a sensitiveness to impact (determined by UN test series 3 (a) (ii)) of 40 J or less and/or a sensitiveness to friction (determined by test series 3 (b) (i)) of 360 N or less.

Such substances may be classified in other hazard classes (e.g. as flammable solids, oxidizing solids, corrosive to metals) or even not at all. Information about such properties should be indicated in the dossier as well.

1 **R.7.1.11.1 Explosives**

2 Definition

3 The following definitions are provided in CLP Annex I, section 2.1.1:

4 *An explosive substance or mixture is a solid or liquid substance or mixture of substances which is in*
5 *itself capable by chemical reaction of producing gas at such a temperature and pressure and at*
6 *such a speed as to cause damage to the surroundings. Pyrotechnic substances are included even*
7 *when they do not evolve gases.*

8
9 *A pyrotechnic substance or mixture is a substance or mixture of substances designed to produce an*
10 *effect by heat, light, sound, gas or smoke or a combination of these as the result of non-detonative*
11 *self-sustaining exothermic chemical reactions.*

12
13 *An unstable explosive is an explosive substance or mixture which is thermally unstable and/or too*
14 *sensitive for normal handling, transport and use.*

15
16 *An explosive article is an article containing one or more explosive substances or mixtures.*

17
18 *A pyrotechnic article is an article containing one or more pyrotechnic substances or mixtures.*

19
20 *An intentional explosive is a substance, mixture or article which is manufactured with a view to*
21 *producing a practical, explosive or pyrotechnic effect.*

22
23 Organic Peroxides and Self Reactive Substances may also have explosive properties and should be
24 screened. See chapter R.7.1.11.3 for Organic peroxides and chapter R.7.1.11.2 for Self Reactive
25 Substances and Mixtures.

26 Classification criteria and relevant information

27 Substances, mixtures and articles of this class are classified as an unstable explosive on the basis of
28 the flowchart in Annex I to CLP Regulation, Figure 2.1.2 . The test methods are described in Part I
29 of the UN Recommendations on the Transport of Dangerous Goods, Manual of Tests and Criteria
30 and also in Section A.14 of Regulation (EC) No 440/2008.

31 REACH applies to individual substances in mixtures. Let's assume that we have a mixture of
32 potassium chlorate (75 %) and dodecanol (25 %). REACH addresses the individual substances
33 which by themselves do not have explosive properties, but CLP Regulation addresses the mixture
34 which would probably be explosive. Therefore, for explosive properties the REACH requirements
35 are equivalent to the CLP requirements when determining the classification. The only difference
36 being that REACH applies to individual substances only, whereas CLP also addresses mixtures of
37 substances.

38 Explosives, which are not classified as an unstable explosive, shall be classified in one of the six
39 divisions referred to in paragraph 2.1.2.2 of Annex 2.1 to the CLP Regulation, based on the results
40 of the tests laid down in Table 2.1.1 on test Series 2 to 8 in Part I of the UN Recommendations on
41 the Transport of Dangerous Goods, Manual of Tests and Criteria. If explosives are unpackaged or
42 repacked in packaging other than the original or similar packaging, they must be retested. If a
43 substance gives a positive result in any of the test series 1 or 2 this should be mentioned, even if it
44 would not be classified as an explosive in test series 6.

45

The test methods used for deciding on provisional acceptance into the class of explosives are grouped into four series, numbered 1 to 4 (see CLP Annex I, Figure 2.1.2).

It may be important for the safety of testers that certain tests, using small amounts of material, be conducted first before proceeding to test with larger quantities. To start the testing procedure with test series 3 is highly recommended, because these tests involve relatively small sample sizes, which reduces the risk to test personnel.

Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

Column 2 of REACH Annex VII provides the following specific rules for adaptation of the standard information requirement for explosive properties.

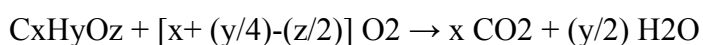
The study does not need to be conducted if:

- *there are no chemical groups associated with explosive properties present in the molecule, or*
- *the substance contains chemical groups associated with explosive properties which include oxygen and the calculated oxygen balance is less than -200, or*
- *the organic substance or a homogenous mixture of organic substances contains chemical groups associated with explosive properties, but the exothermic decomposition energy is less than 500 J/g and the onset of exothermic decomposition is below 500 °C, or*
- *for mixtures of inorganic oxidising substances (UN Division 5.1) with organic materials, the concentration of the inorganic oxidising substance is:*
 - *less than 15 %, by mass, if assigned to UN Packaging Group I (high hazard) or II (medium hazard),*
 - *less than 30 %, by mass, if assigned to UN Packaging Group III (low hazard).*

Note: Neither a test for propagation of detonation nor a test for sensitivity to detonative shock is required if the exothermic decomposition energy of organic materials is less than 800 J/g.

Note on the use of the Oxygen Balance:

The oxygen balance is calculated for the chemical reaction:



Using the formula:

$$\text{Oxygen balance} = -1600 [2x + (y/2) - z] / \text{molecular weight};$$

The oxygen balance was developed for compounds containing only (multiple) nitrate groups. Extending its use to molecules with other (oxygen containing) groups should be done with care. As an example the presence of hydroxyl-groups will strongly affect the oxygen balance towards higher values, whereas this group does not contribute to explosive properties. In addition the presence of for instance halogens tends to decrease the flammability and explosivity but this is not accounted for.

1 **Waiving possibilities according to Annex XI to REACH**

2 **USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM**
3 **EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS**
4 **REFERRED TO IN ARTICLE 13 (3) OF REACH**

5 Data that satisfies the REACH Annex XI requirements are not available. Literature data should not
6 be used, because factors such as particle size and impurities may have great influence on the
7 explosive behaviour of substances.

8 **WEIGHT OF EVIDENCE**

9 Application of weight of evidence is possible with substances where explosive properties can
10 clearly be excluded. Weight of evidence should be accompanied with extensive and reliable
11 literature references.

12 **(Q)SAR**

13 There is currently no QSPR/(Q)SAR software known with sufficient accuracy and reliability to
14 assist in assessing (potential) explosive properties. DSC testing is cheap and fast and is strongly
15 recommended to identify potential hazards connected with the substance.

16 A number of recent publications have dealt with the QSPR modelling of flammability (Gharagheizi,
17 2008, 2009a), particularly with experimental data extracted from the robust consolidated DIPPR
18 database. So far as is known, no software is available for the prediction of flammability limits.

19 **GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH**

20 Testing may be waived if there are no chemical groups associated with explosive properties present
21 in the molecule. Examples of groups which may indicate explosive properties are given in the table
22 below, which is taken from table A6.1 in Appendix 6 of the UN Recommendations on the Transport
23 of Dangerous Goods, Manual of Tests and Criteria.

24 Table xxxxx: Examples of chemical groups indicating explosive properties in organic materials.

Structural Feature	Examples
C-C unsaturation	Acetylenes, acetylides, 1,2-dienes
C-Metal, N-Metal	Grignard reagents, organo-lithium compounds
Contiguous nitrogen atoms	Azides, aliphatic azo compounds, diazonium salts, hydrazines, sulphonylhydrazides
Contiguous oxygen atoms	Peroxides, ozonides
N-O	Hydroxylamines, nitrates, nitro compounds, nitroso compounds, N-oxides, 1,2-oxazoles
N-halogen	Chloramines, fluoroamines
O-halogen	Chlorates, perchlorates, iodosyl compounds

Note on the use of the above table: this table is not exhaustive, other references may list more high functional groups with potential explosive properties.

Application of read across is not possible.

TESTING IS TECHNICALLY NOT POSSIBLE

Testing for explosives may be omitted if it is technically not possible to conduct the study as a consequence of the properties of the substance.

Further waiving possibilities

A substance or mixture which is not itself an explosive but which can form an explosive atmosphere of gas, vapor or dust is not included in this class.

Impurities; uncertainties

Small amounts of other compounds may enhance or suppress the chemical reaction that gives the explosive property to a substance. Therefore impurities may considerably influence the explosive properties of a substance. For further information please refer to the paragraph addressing uncertainties in test methods in chapter R.7.1.1.4.

How to conclude on the DSD classification

For DSD explosives are substances and preparations which may explode under the effect of flame or which are more sensitive to shocks or friction than dinitrobenzene.

Reclassification of substances classified as explosive according to DSD:

Under the regime of the old DSD, testing of explosive properties was achieved by performing test A.14. For classification purposes under the CLP Regulation this test is not relevant. Testing according to the CLP Regulation is the same as that described in Part I of the UN Recommendations on the Transport of Dangerous Goods, Manual of Tests and Criteria. This is why

the translation table of Annex VII of the CLP Regulation states that there is no direct translation possible for classification from (E, R2) and (E, R3) to CLP criteria.

Therefore, if the screening procedure of section 2.1.4.2 of the CLP Regulation identifies a substance or mixture to be a potential explosive, appropriate data are required for classification.

Moreover, if data from performing test A.14 or the UN Test series 3 tests 3a or 3b indicate that a substance is sensitive to impact or friction such information should be provided in the safety data sheet.

Endpoint specific information in the registration dossier/in IUCLID

Material and methods

- reference to the standard and the test method applied;
- description of the substance that was tested.

Results and discussion

- If testing is waived, the reasons for waiving must be documented in the dossier;
- If testing is not waived then the tests done according to the UN Test Manual and the outcome (explosive or not explosive) must be documented in the dossier. The mechanical sensitivity test according to UN Test series 3a and 3b must be done and documented if UN Test series 1 or 2 give a positive result. If data according to test A.14 are available, then the results can be used instead of UN Test series 3a and 3b.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on explosiveness can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.14	VII 7.11	Explosiveness	E.4.15	3.12

Further information / references

Further information about classification and testing for explosives can be found in the *Guidance on the application of CLP criteria*, section 2.2.

Gharagheizi F. Quantitative structure-property relationship for prediction of the lower flammability limit of pure compounds. *Energy & Fuels* 22 (2008) 3037-3039.

Gharagheizi F. A new group contribution-based model for estimation of lower flammability limit of pure compounds. *J. Haz. Mat.* 170 (2009a) 595-604.

R.7.1.11.2 Self-reactive substances and mixtures

Definition

The definition of a self-reactive substance is given in CLP Regulation Annex I, section 2.8.1.

Self-reactive substances or mixtures are thermally unstable liquid or solid substances or mixtures liable to undergo a strongly exothermic decomposition even without participation of oxygen (air). This definition excludes substances or mixtures be tested for classification according to this part as explosives, organic peroxides or as oxidising.

A self-reactive substance or mixture is regarded as possessing explosive properties when in laboratory testing the formulation is liable to detonate, to deflagrate rapidly or to show a violent effect when heated under confinement.

Background information and guidance on the definition is given in the *Guidance on the Application of the CLP Criteria*, sections 2.9.1 and 2.9.2.

Classification criteria and relevant information

Classification principles are given in CLP Regulation Annex I, sections 2.8.2 and 2.8.4.

Background information and guidance on relevant aspects regarding the classification is given in the *Guidance on the Application of the CLP Criteria*, sections 2.9.3, 2.9.5 and 2.9.6.

Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

Only self-reactive substances, as defined in section definition, have to be tested according to the United Nations Manual of Tests and Criteria, Part II test series A - H.

CLP Annex I provides the following specific rules for adaptation of the standard information requirement for self-reactive substances and mixtures.

Any self-reactive substance or mixture shall be considered for classification in this class as a self-reactive substance or mixture unless:

(a) *they are explosives, according to the criteria given in 2.1;*

(b) *they are oxidising liquids or solids, according to the criteria given in 2.13 or 2.14, except that mixtures of oxidising substances, which contain 5 % or more of combustible organic substances shall be classified as self-reactive substances according to the procedure defined in the 2.8.2.2 below;*

(c) *they are organic peroxides, according to the criteria given in 2.15;*

(d) *their heat of decomposition is less than 300 J/g; or*

(e) *their self-accelerating decomposition temperature (SADT) is greater than 75 °C for a 50 kg package.*

(See UN Recommendations on the Transport of Dangerous Goods, Manual of Tests and Criteria, sub-sections 28.1, 28.2, 28.3 and Table 28.3.)

1 **Waiving possibilities according to Annex XI to REACH**

2 **USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM**
3 **EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS**
4 **REFERRED TO IN ARTICLE 13 (3) OF REACH**

5 A number of already tested and classified substances and mixtures are listed in United Nations
6 Recommendations on the Transport of Dangerous Goods, section 2.4.2.3.2.3. Available information
7 may originate from the classification for transport. More details are described in the Guidance on
8 the Application of the CLP Criteria, sections 1.7.2.1 and 2.9.5.

9 **WEIGHT OF EVIDENCE**

10 For the determination of the self-reactive substances and mixtures, weight of evidence is not
11 possible.

12 **(Q)SAR**

13 At present (Q)SAR is generally not applicable for determination of self-reactives. Application of
14 (Q)SAR is not possible.

15 **GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH**

16 At present grouping and read-across are not applicable.

17 **TESTING IS TECHNICALLY NOT POSSIBLE**

18 A few of substances can, for safety reasons, only be handled and tested in diluted form, see the
19 substances and mixtures listed in UN TDG, section 2.4.2.3.2.3.

20 **Further waiving possibilities**

21 Not foreseen.

22 Impurities; uncertainties

23 Minor impurities can have an influence on the thermal stability. Background information and
24 guidance on these aspects is given in the *Guidance on the Application of the CLP Criteria*, section
25 2.9.3.3.

26 How to conclude on the DSD classification

27 In the DSD self-reactive substances are not covered. They may be classified in other DSD classes
28 (e.g. explosive substance, flammable solid or liquid). However, in the CLP Regulation self-reactive
29 substances are classified as Type A (explosive), Type B (self-reactive substance and explosive) and
30 Types C-G (self-reactive substance). See also the *Guidance on the Application of the CLP Criteria*,
31 section 2.9.5.

32 What information is required in the registration dossier in IUCLID

33 **Material and methods**
34

See UN MTC, Part II, classification procedures and test series A-H.

Results and discussion

The following data on self-reactive substances should be submitted:

- type of self-reactive substance;
- decomposition energy (value and method of determination);
- SADT (Self accelerating decomposition temperature);
- detonation properties (Yes/Partial/No);
- deflagration properties (Yes rapidly/Yes slowly/No);
- effect of heating under confinement (Violent/Medium/Low/No);
- explosive power if applicable (Not low/Low/None);

For assigning the type of self-reactive substance, the list of currently assigned self-reactive substances according to the 2.4.2.3.2.3 of the UN RTDG can be used, in case the assignment was based on test according to the UN MTC. The relevant underlying test data may be collected from the respective UN documents from the UN committee of experts on the transport of dangerous goods, from test reports produced by competent authorities or by industry, or from other reliable sources.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on flammability can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.13	VII 7.10	Flammability	E.4.14	3.11

Further information / references

Background information and guidance on classification testing, additional testing and available information is given in the *Guidance on the Application of the CLP Criteria*, section 2.9.

R.7.1.11.3 Organic peroxides

Definition

The definition of an organic peroxide is given in CLP Annex I, section 2.15.1:

Organic peroxide means a liquid or solid organic substance which contains the bivalent -O-O- structure and as such is considered a derivative of hydrogen peroxide, where one or both of the hydrogen atoms have been replaced by organic radicals. The term organic peroxide includes organic peroxide mixtures (formulations) containing at least one organic peroxide. Organic peroxides are thermally unstable substances or mixtures, which can undergo exothermic self-accelerating decomposition. In addition, they can have one or more of the following properties:

- (i) Be liable to explosive decomposition;*
- (ii) Burn rapidly;*
- (iii) Be sensitive to impact or friction;*
- (iv) React dangerously with other substances.*

An organic peroxide is regarded as possessing explosive properties when in laboratory testing the mixture (formulation) is liable to detonate, to deflagrate rapidly or to show a violent effect when heated under confinement.

Background information and guidance on the definition is given in *Guidance on the Application of the CLP Criteria*, sections 2.14.1 and 2.14.2.

Classification criteria and relevant information

The Classification principles are given in CLP Annex I, sections 2.15.2 and 2.15.4.

Background information and guidance on relevant aspects regarding the classification is given in *Guidance on the Application of the CLP Criteria*, sections 2.14.3, 2.14.4, 2.14.6, 2.14.7 and 2.14.8.

Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

Only organic peroxides, as defined in the CLP, Annex I, section 2.15.1 definition, have to be tested according to the United Nations Manual of Tests and Criteria, Part II test series A - H.

The study does not need to be conducted if:

- *the substance or mixture contains:*

- (a) not more than 1.0% available oxygen from the organic peroxides when containing not more than 1.0% hydrogen peroxide; or*
- (b) not more than 0.5% available oxygen from the organic peroxides when containing more than 1.0% but not more than 7.0% hydrogen peroxide.*

NOTE:

The available oxygen content (%) of an organic peroxide mixture is given by the formula:

$$16 \times \sum_i^n \left(\frac{n_i \times c_i}{m_i} \right)$$

where:

n_i = number of peroxygen groups per molecule of organic peroxide i ;

1 c_i = concentration (mass %) of organic peroxide i ;

2 m_i = molecular mass of organic peroxide i .

3 **Waiving possibilities according to Annex XI to REACH**

4 **USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM**
5 **EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS**
6 **REFERRED TO IN ARTICLE 13 (3) OF REACH**

7 A number of already tested and classified substances and mixtures are listed in United Nations
8 Recommendations on the Transport of Dangerous Goods, 2.5.3.2.4.

9 Available information may especially originate from the classification for transport. In DSD organic
10 peroxides were classified as oxidizing substances, by definition. More details are described in the
11 *Guidance on the Application of the CLP Criteria*, sections 1.7.2.1 and 2.14.6.

12 **WEIGHT OF EVIDENCE**

13 For the determination of the organic peroxides, weight of evidence is not possible.

14 **(Q)SAR**

15 At present (Q)SAR is generally not applicable for organic peroxides. Application of (Q)SAR is not
16 possible.

17 **GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH**

18 At present grouping and read across are not applicable.

19 **TESTING IS TECHNICALLY NOT POSSIBLE**

20 A number of substances can, for safety reasons, only be handled and tested in diluted form, see the
21 substances and mixtures listed in UN TDG, 2.5.3.2.4.

22 **Further waiving possibilities**

23 Not foreseen.

24 Impurities; uncertainties

25 Minor impurities can have an influence on the thermal stability. Background information and
26 guidance on these aspects is given in *Guidance on the Application of the CLP Criteria*, section
27 2.14.4.

28 How to conclude on the DSD classification

29 In the DSD organic peroxides are classified as oxidizing substances and a few of them as having
30 explosive properties. However, in the CLP Regulation organic peroxides are classified as Type A
31 (explosive), Type B (organic peroxide and explosive) and Types C-G (organic peroxide). See also
32 *Guidance on the Application of the CLP Criteria*, section 2.14.6.

Endpoint specific information in the registration dossier/in IUCLID**Material and methods**

- See UN MTC, Part II, classification procedures and test series A-H.

Results and discussion

The following data of organic peroxides should be submitted:

- type of organic peroxide;
- SADT (Self accelerating decomposition temperature);
- detonation properties (Yes/Partial/No);
- deflagration properties (Yes rapidly/Yes slowly/No);
- effect of heating under confinement (Violent/Medium/Low/No);
- explosive power, if applicable (Not low/Low/None).

For assigning the Type of organic peroxide, the list of currently assigned organic peroxides according 2.5.3.2.4 of the UN RTDG can be used, in case the assignment was based on a test according to the UN MTC. The relevant underlying test data may be collected from the respective UN documents from the UN committee of experts on the transport of dangerous goods, from test reports produced by competent authorities or by industry, or from other reliable sources (such as e.g. the dedicated database ‘DATATOP’).

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on flammability can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.13	VII 7.10	Flammability	E.4.14	3.11

Further information / references

Background information and guidance on classification testing, additional testing and available information is given in the *Guidance on the Application of the CLP Criteria*, section 2.14.

Data from the ‘DATATOP’ database can be obtained from the gatekeeper of this data base TNO, Department Energetic Materials, Lange Kleiweg 137, 2288GJ, Rijswijk The Netherlands.

R.7.1.12 SELF-IGNITION TEMPERATURE

The terminology used in Annex VII of REACH is not very precise. Therefore, some guidance in interpretation appears necessary:

- For liquids and gases, the term ‘**auto-ignition**’ instead of ‘self-ignition’ is generally used. Auto-ignitability is of high importance for the assignment of temperature classes in explosion protection (i. e. ATEX in Europe) of plants and equipment.
- For solids and liquids absorbed on a large surface, **self-heating** may occur by reaction with air with subsequent ignition. According to the CLP Regulation, Annex I, section 2.11, a self-heating substance or mixture is a liquid or solid substance or mixture, other than a pyrophoric liquid or solid, which, by reaction with air and without energy supply, is liable to self-heat; this substance or mixture differs from a pyrophoric liquid or solid in that it will ignite only when in large amounts (kilograms) and after long periods of time (hours or days). Therefore solids are considered under self heating substances in the chapter below.

Table x: Assignment of CLP hazard classes to the information requirement ‘Self ignition temperature’ according to REACH, Annex VII and the Test Method Regulation.

REACH Regulation (EC) No. 1907/2006 (the no. in brackets is the respective no. in the table of REACH Annex VII)	Related hazard class according to the CLP Regulation (the no. in brackets is the respective chapter no. in Annex I to CLP)	Chapter in revised R.7(a) guidance	Test method according to the Test Method Regulation 440/2008	Test method according to the CLP Regulation	Chapter in the Guidance on the Application of the CLP Criteria (ex RIP 3.6)
Self ignition temperature (7.12)	For gases and liquids	7.1.12.1	A.15 Auto-ignition temperature (liquids and gases)	/	/
	For solids	7.1.12.2, 7.1.10.8	A.16 Relative self-ignition temperature for solids	/	Section 2.11

R.7.1.12.1 Auto- ignitionType of property

For liquids and gases, the term ‘**auto-ignition**’ instead of ‘self-ignition’ is generally used. Auto-ignitability is of high importance for the assignment of temperature classes in explosion protection (i. e. ATEX in Europe) of plants and equipment. In this chapter, only the **auto-ignition** phenomena will be discussed.

1 Definition

2 The degree of auto-ignitability is expressed in terms of the auto-ignition temperature. The auto-
3 ignition temperature is the lowest temperature at which the test substance will ignite when mixed
4 with air under the conditions defined in the test method.

5
6 Test method(s)

7 Method A.15 of Regulation EC 440/2008 (Auto-ignition temperature) should be used for testing
8 which references several national and international standards. The test procedure is applicable to
9 gases, liquids and vapours which, in the presence of air, can be ignited by a hot surface. Where
10 standards are applicable, the use of the most recent updates is advised.
11

12 Adaptation of the standard testing regime

13 **Waiving possibilities according to column 2 of Annex VII to REACH**

14 Column 2 of REACH Annex VII provides the following specific rules for adaptation of the standard
15 information requirement for self-ignition temperature.

16 *The study does not need to be conducted:*

- 17 – *if the substance is explosive or ignites spontaneously with air at room temperature; or*
18 – *for liquids non flammable in air, e.g. no flash point up to 200 °C; or*
19 – *for gases having no flammable range, or*
20 – *for solids, if the substance has a melting point ≤ 160 °C, or if preliminary results exclude self-*
21 *heating of the substance up to 400 °C.*

22 This means:

23 For gases:

24 Only gases classified as flammable according to the CLP Regulation have to be considered.

25 For liquids:

26 The auto-ignition temperature should be determined according to Directive EC 440/2008, method
27 A.15. No data are required for liquids classified as

- 28 • pyrophoric; or
29 • explosive, unstable or division 1.1 to 1.6; or
30 • organic peroxide; or
31 • self-reactive substance.

32 Further, the auto-ignition temperature does not have to be determined for liquids having no flash
33 point up to 200 °C. In practice, liquids with a boiling point above 350 °C will not have a flash point
34 below 200 °C. Therefore, determination of the auto-ignition temperature is not necessary in such
35 cases if the flash point is not known.

WAIVING POSSIBILITIES ACCORDING TO ANNEX XI TO REACH

USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS REFERRED TO IN ARTICLE 13 (3) OF REACH

The use of existing experimental data is possible if they have been determined by certified institutions. Further, the auto-ignition temperature does not have to be determined experimentally if conclusive and consistent literature data are available.

WEIGHT OF EVIDENCE

For the determination of the auto-ignition temperature, the weight of evidence approach is not possible.

(Q)SAR

For the determination of the auto-ignition temperature, (Q)SAR approaches are strongly discouraged for the purpose of classification/ risk assessment.

GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH

Read across is generally not possible for the determination of the auto-ignition temperature. Interpolation within homologous series may be used. However, it is not possible to read across from methyl compounds to ethyl and propyl compounds and vice versa.

TESTING IS TECHNICALLY NOT POSSIBLE

Substances which decompose below room temperature or which react vigorously with moisture may be difficult to test. In such cases, the test may be waived due to technical reasons.

Further waiving possibilities

Not foreseen.

Impurities; uncertainties

The auto-ignition temperature can be considerably reduced by the presence of catalytic impurities.

Endpoint specific information in the registration dossier / in IUCLID

Material and methods

- description of the apparatus or reference to the standard or the test method applied;
- quantity of sample used.

Results and discussion

- The value or the range of the auto-ignition temperature;

For liquids/gases: observations (e.g decomposition with air, reactions with moisture, etc.)

For solids see the below R.7.1.12.2.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on auto flammability can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.12	VII 7.12	Auto flammability	E.4.13	3.10

R.7.1.12.2 Self-heating substances

For solids and liquids absorbed on a large surface, **self-heating** may occur by reaction with air with subsequent ignition. According to the CLP Regulation Annex I, section 2.11 the following definition is provided:

A self-heating substance or mixture is a liquid or solid substance or mixture, other than a pyrophoric liquid or solid, which, by reaction with air and without energy supply, is liable to self-heat; this substance or mixture differs from a pyrophoric liquid or solid in that it will ignite only when in large amounts (kilograms) and after long periods of time (hours or days).

The ECHA *Guidance on the Application of the CLP Criteria* gives in Chapter 2.11 detailed information on the self-heating property, the CLP-classification, the relevant test method and the relation to the DSD and the transport of dangerous goods regulations.

See section R.7.1.10.8 of this guidance document for further details and information.

R.7.1.13 OXIDISING PROPERTIES

Some of the information requirements according to REACH Annex VII were phrased such that they correspond to ‘indications of danger’ as given in Annex II of DSD. For substances, classification and labelling according to the CLP Regulation has been mandatory since December 1, 2010 (and will become mandatory for mixtures (preparations) from June 1 2015, when the DSD will be repealed). Consequently, information requirements on oxidising properties are inherently covered by classification of the substance according to the CLP Regulation. However, the physical hazards according to CLP Regulation are structured completely differently from the physico-chemical properties according to DSD (and therefore also REACH, Annex VII). This means that for some of the CLP hazard classes an unambiguous assignment to one of the headlines (information requirements) in Annex VII to REACH is not possible. The assignment of hazard classes to the headline ‘Oxidising properties’ as shown in table below must therefore only be understood as a means to structure this document in accordance with Annex VII to REACH.

Table x: Assignment of CLP hazard classes to the information requirement ‘Oxidising properties’ according to REACH, Annex VII and correlation between the Test method Regulation

and the test method according to CLP and supporting link with the Guidance on the application of the CLP Criteria.

REACH Regulation (EC) No. 1907/2006 (the no. in brackets is the respective no. in the table in Annex VII to REACH)	Related hazard class according to CLP Regulation (EC) No. 1272/2008 (the no. in brackets is the respective chapter no. in Annex I to CLP)	Chapter in revised R.7(a) guidance	Test method according to the Test Method Regulation 440/2008	Test method according to the CLP Regulation	Chapter in the Guidance on the Application of the CLP Criteria (ex RIP 3.6)
Oxidising properties (7.13)	Oxidising gases (2.4)	7.1.13.1	/	ISO 10156	2.5
	Oxidising liquids (2.13)	7.1.13.2	A.21 Oxidising properties (liquids)	UN O.2	2.13
	Oxidising solids (2.14)	7.1.13.3	A.17 Oxidising properties (solids)	UN O.1	2.13

R.7.1.13.1 Oxidising gases

Definition

Oxidising gas means any gas or gas mixture which may, generally by providing oxygen, cause or contribute to the combustion of other material more than air does (Annex I to CLP, section 2.4.1).

The criteria '*more than air does*' is further defined in a Note under Table 2.4.1 in Section 2.4.1 as '*having an oxidising power greater than 23.5 % as determined by a method specified in ISO 10156 as amended*'.

Classification criteria and relevant information

All oxidising gases are classified as Oxidising gas, Category 1 (Ox. Gas 1, H270). Detailed guidance on the classification criteria and the test method(s) can be found in the *Guidance on the application of the CLP Criteria*, section 2.5.

Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

Column 2 of REACH Annex VII provides the following specific rules for adaptation of the standard information requirement for oxidising properties.

The study does not need to be conducted if:

- the substance is explosive, or

- *the substance is highly flammable, or*
- *the substance is an organic peroxide, or*
- *the substance is incapable of reacting exothermically with combustible materials, for example on the basis of the chemical structure (e.g. organic substances not containing oxygen or halogen atoms and these elements are not chemically bonded to nitrogen or oxygen, or inorganic substances not containing oxygen or halogen atoms).*

The full test does not need to be conducted for solids if the preliminary test clearly indicates that the test substance has oxidising properties.

Note that as there is no test method to determine the oxidising properties of gaseous mixtures, the evaluation of these properties must be realised by an estimation method based on the comparison of the oxidising potential of gases in a mixture with that of the oxidising potential of oxygen in air.

The study does not need to be conducted if the gas:

- is classified as flammable; or
- is incapable of reacting exothermically with combustible materials, for example on the basis of its chemical structure that does not contain oxygen or halogen atoms.

Waiving possibilities according to Annex XI to REACH

USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS REFERRED TO IN ARTICLE 13 (3) OF REACH

There are not many gases that are oxidising. Most oxidising gases are identified as such in the UN-RTDG and in ISO 10156:2010 *Gas cylinders - Gases and gas mixtures: - Determination of fire potential and oxidizing ability for the selection of cylinder valve outlets*.

No test is needed for the oxidising gases listed in ISO 10156.

WEIGHT OF EVIDENCE

There is no known scientific literature that refers to test results for gases that are not classified in ISO 10156 nor in the UN-RTDG.

(Q)SAR

At present (Q)SAR is generally not applicable for the determination of oxidising limits of gases. Application of (Q)SAR is not possible. However, assessment of the chemical structure may be used to exclude oxidising behaviour of a substance. Possibly, this relation could be exploited in the development of future QSPR methods.

GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH

At present grouping and read across are not applicable.

TESTING IS TECHNICALLY NOT POSSIBLE

In this case testing should always be possible.

Further waiving possibilities

Not foreseen.

Impurities; uncertainties

The normal level of impurities in the technical grade of oxidising gases does not impact the result of the test. Tests should be performed with the lowest concentration of impurities in the gas encountered in the normal manufacturing process and the moisture content should be less than or equal to 0.01 %.

How to conclude on the DSD classification

All gases with a positive test result according to the test method described in ISO 10156 are classified ‘Oxidising O, R8’.

Endpoint specific information in the registration dossier/in IUCLID

Material and methods

- reference to the standard applied.

Results and discussion

- If the test is positive indicate that it is ‘more oxidising than air’.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on oxidising properties can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.15	VII 7.13	Oxidising properties	E.4.16	3.13

Further information / references

The test method is described in ISO 10156. The test is qualitative. If reaction is observed during the test, the gas to be evaluated is more oxidizing than air.

For several gases, a ‘coefficient of oxygen equivalency’ (Ci) has been deduced from the explosion ranges observed during the tests. The Ci factors are listed in ISO 10156 along with the list of oxidising gases.

1 **R.7.1.13.2 Oxidising liquids**

2 Definition

3 The following definition of oxidising liquids is provided in CLP Annex I, section 2.13.1:

4 *Oxidising liquid means a liquid substance or mixture which, while in itself not necessarily*
5 *combustible, may, generally by yielding oxygen, cause, or contribute to, the combustion of other*
6 *material.*

7 Classification criteria and relevant information

8 According to the CLP Regulation, a liquid is classified as an Oxidising Liquid if, in testing
9 according to the O.2 test method of the UN Manual of Tests and Criteria (Part III, Section 34) it is
10 at least as oxidising as a 65 % aqueous solution of nitric acid. The CLP Regulation has three
11 categories for Oxidising Liquids. The category is also determined through the O.2 test method, by
12 comparison to various reference oxidisers.

13 In the DSD, the A.21 test method of Regulation (EC) 440/2008 is used for the assessment of
14 oxidising properties of liquids. This method is in principle identical to the O.2 test method of the
15 UN Manual of Tests and Criteria used in the CLP Regulation. However, the DSD does not make
16 any division corresponding to the categories of the CLP, and therefore only one reference substance
17 is used in the A.21 test method. Since the CLP Regulation method is used for classification of
18 substances, it is strongly advisable to use the O.2 test method instead of the A.21 test method. This
19 is because the O.2 test method will also give more detailed information on the oxidising behaviour
20 of a substance (or mixture), since more reference mixtures are used.

21 Adaptation of the standard testing regime

22 **Waiving possibilities according to column 2 of Annex VII to REACH**

23 Column 2 of REACH Annex VII provides the following specific rules for adaptation of the standard
24 information requirement for oxidising properties.

25 *The study does not need to be conducted if:*

- 26 – *the substance is explosive, or*
- 27 – *the substance is highly flammable, or*
- 28 – *the substance is an organic peroxide, or*
- 29 – *the substance is incapable of reacting exothermically with combustible materials, for*
30 *example on the basis of the chemical structure (e.g. organic substances not containing*
31 *oxygen or halogen atoms and these elements are not chemically bonded to nitrogen or*
32 *oxygen, or inorganic substances not containing oxygen or halogen atoms).*

33 *The full test does not need to be conducted for solids if the preliminary test clearly indicates that the*
34 *test substance has oxidising properties.*

35 *Note that as there is no test method to determine the oxidising properties of gaseous mixtures, the*
36 *evaluation of these properties must be realised by an estimation method based on the comparison of*
37 *the oxidising potential of gases in a mixture with that of the oxidising potential of oxygen in air.*

The first indent states that explosive substances should not be tested for oxidising properties. For instance, organic substances with oxidising functional groups may be explosive and should first undergo the screening procedures for explosive properties in Annex 6 of the UN Manual of Tests and Criteria to rule out possible explosive behaviour. Such substances may also be thermally unstable and show self-reactive behaviour. Substances that have been classified as Explosives according to the CLP Regulation or have been assigned risk phrases R2 or R3 according the DSD, should normally not be tested for oxidising properties, since they are known to be explosive.

The second indent states that highly flammable substances do not have to be tested for oxidising properties. While it is not very clear what ‘highly flammable’ means in this case, liquids that have a low flash point, or which are pyrophoric, are rarely oxidising. This implies that liquids classified as Flammable Liquids category 1 or 2, or as Pyrophoric Liquids, according to the CLP Regulation, normally do not need to be tested for oxidising properties. This corresponds to classification with risk phrases R12, R11 or R17 according to the DSD. If they contain oxidising functional groups, such substances may instead show self-reactive or explosive behaviour.

The third indent states that organic peroxides should not be tested for oxidising properties. Organic peroxides are distinguished by their chemical structure, and should be treated according to the procedures for the hazard class Organic Peroxides of the CLP Regulation, see Section R.7.1.10.10 of this document.

Waiving according to the fourth indent relies on the absence of particular molecular structural features. The wording is more precise in Section 2.13.4 of Annex I to the CLP Regulation, which is in principle the same as the wording as in Section 6 of Appendix 6 to the UN Manual of Tests and Criteria.

According to 2.13.4.1 of Annex I to the CLP Regulation, an organic liquid does not have to be assessed for oxidising properties if:

- (i) *the substance does not contain oxygen, fluorine or chlorine; or*
- (ii) *the substance contains oxygen, fluorine or chlorine and these elements are chemically bonded only to carbon or hydrogen.*

For inorganic liquids, assessment of oxidising properties does not have to be done if the substance does not contain any oxygen or halogen atoms, according to section 2.13.4.2 of Annex I to the CLP Regulation.

Waiving possibilities according to Annex XI to REACH

USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS REFERRED TO IN ARTICLE 13 (3) OF REACH

The O.2 test method of the UN Manual of Tests and Criteria is also used for classification according to the UN Model Regulations on the Transport of Dangerous Goods, and consequently also in the various regulations on transport of dangerous goods e.g. ADR and RID. A liquid that has been classified as belonging to Division 5.1 according to the regulations on transport of dangerous goods on the basis of results from the O.2 test method, is an Oxidising Liquid according to the criteria of the CLP Regulation.

1 **WEIGHT OF EVIDENCE**

2 For the determination of oxidising properties, weight of evidence is not possible.

3 **(Q)SAR**

4 At the time of writing, no reliable (Q)SAR-methods exist for sufficiently accurate predictions of
5 oxidising properties. As explained above, however, assessment of the chemical structure may be
6 used to exclude oxidising behaviour of a substance. Possibly, this relation could be exploited in the
7 development of future QSPR-methods.

8 **GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH**

9 At present grouping and read across are not applicable.

10 **TESTING IS TECHNICALLY NOT POSSIBLE**

11 Some oxidising substances may decompose when heated. Substances may occasionally react with
12 cellulose in other ways than through oxidation of the cellulose (e.g. through breaking chemical
13 bonds within the cellulose). See also 2.13.4.4 of Annex I to the CLP Regulation.

14 **Further waiving possibilities**

15 Not foreseen.

16

17 Impurities; uncertainties

18 Minor impurities will usually not influence the test, unless they are very strong oxidisers. Expert
19 judgement should be used to determine whether impurities may have an effect.

20 A few substances may show other reactions than pure oxidation of the cellulose, or may
21 decompose. If this is suspected, expert judgement should be sought. See also 2.13.4.4 of Annex I to
22 the CLP Regulation.

23 How to conclude on the DSD classification

24 Any substance classified as an Oxidising Liquid according to the CLP-criteria should normally be
25 classified with risk phrase R8 or R9 according to the DSD. The DSD-criteria for classification with
26 risk phrase R9 are not very precise, but if the CLP classification is Category 1, the substance should
27 be classified with risk phrase R9 if the reaction with cellulose is violent, e.g. if spontaneous ignition
28 occurs in the test.

29 Endpoint specific information in the registration dossier/in IUCLID

30 **Material and methods**

- 31 • description of the apparatus and dimensions or reference to the standard or the test method
32 applied;

33

34 **Results and discussion**

- 35 • indicate the results of the spontaneous ignition test;
36 • indicate the mean pressure rise time for the test substance;
37 • indicate the mean pressure rise time for the reference substance(s);

- interpretation of results.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on oxidising properties can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.15	VII 7.13	Oxidising properties	E.4.16	3.13

Further information / references

The ECHA guidance document *Guidance on the Application of the CLP Criteria* gives in Chapter 2.13 detailed information on the oxidising property, the CLP-classification, the O.2-test method and the relation to the DSD and the transport of dangerous goods regulations.

R.7.1.13.3 Oxidising solids

Definition

An oxidising solid means a solid substance or mixture which, while in itself not necessarily combustible, may, generally by yielding oxygen, cause, or contribute to, the combustion of other material.

Classification criteria and relevant information

According to the CLP Regulation, a solid is classified as an Oxidising Solid if in testing according to the O.1 test method of the UN Manual of Tests and Criteria (Part III, Section 34), it is at least as oxidising as potassium bromate in a 3:7 mixture with cellulose. The test is based on the burning behaviour of a mixture of cellulose and the tested solid. The CLP Regulation has three categories for Oxidising Solids. The category is also determined through the O.1 test method in the UN Manual of Tests and Criteria, by comparison to reference mixtures of cellulose and potassium bromate¹⁰.

In the DSD, the A.17 test method of Regulation (EC) 440/2008 is used for the assessment of oxidising properties of solids. Although the principle of this method is to a large extent the same as that of the O.1 test method of the UN Manual of Tests and Criteria, the experimental set-up and measured quantity differ. Furthermore, the DSD does not make any division corresponding to the categories of the CLP. Since the CLP Regulation is used for classification of substances, it is not advisable to use the A.17 method (which belongs to the DSD classification system). Instead, the

¹⁰ At the time of writing, work is in progress at the UN-level to modify the O.1-test method. This includes changing the reference substance and introducing a gravimetric method for the measurement of the burning rate.

O.1 test method should be used, which will also give more detailed information on the oxidising behaviour of a substance (or mixture), since more reference mixtures are used.

Adaptation of the standard testing regime

Waiving possibilities according to column 2 of Annex VII to REACH

Column 2 of REACH Annex VII provides the following specific rules for adaptation of the standard information requirement for oxidising properties.

The study does not need to be conducted if:

- the substance is explosive, or*
- the substance is highly flammable, or*
- the substance is an organic peroxide, or*
- the substance is incapable of reacting exothermically with combustible materials, for example on the basis of the chemical structure (e.g. organic substances not containing oxygen or halogen atoms and these elements are not chemically bonded to nitrogen or oxygen, or inorganic substances not containing oxygen or halogen atoms).*

The full test does not need to be conducted for solids if the preliminary test clearly indicates that the test substance has oxidising properties.

Note that as there is no test method to determine the oxidising properties of gaseous mixtures, the evaluation of these properties must be realised by an estimation method based on the comparison of the oxidising potential of gases in a mixture with that of the oxidising potential of oxygen in air.

The first indent states that explosive substances should not be tested for oxidising properties. For instance, organic substances with oxidising functional groups may be explosive and should first undergo the screening procedures for explosive properties in Annex 6 of the UN Manual of Tests and Criteria to rule out possible explosive behaviour. Such substances may also be thermally unstable and show self-reactive behaviour. Substances that have been classified as Explosives according to the CLP-regulation or have been assigned risk phrases R2 or R3 according the DSD, should normally not be tested for oxidising properties, since they are known to be explosive.

The second indent states that highly flammable substances do not have to be tested for oxidising properties. While it is not very clear what ‘highly flammable’ means in this case, solids classified as Flammable Solids or as Pyrophoric Solids according to the CLP-regulation are rarely oxidising. This corresponds to classification with risk phrases R11 or R17 according to the DSD. If they contain oxidising functional groups, such substances may instead show self-reactive or explosive behaviour.

The third indent states that organic peroxides should not be tested for oxidising properties. Organic peroxides are distinguished by their chemical structure, and should be treated according to the procedures for the hazard class Organic Peroxides of the CLP-regulation, see Section R.7.1.10.10 of this document.

Waiving according to the fourth indent relies on the absence of particular molecular structural features. The wording is more precise in Section 2.14.4 of Annex I to the CLP-regulation, which is

in principle the same as the wording as in Section 6 of Appendix 6 to the UN Manual of Tests and Criteria.

According to 2.14.4.1 of Annex I to the CLP-regulation, an organic solid does not have to be assessed for oxidising properties if:

- (i) *the substance does not contain oxygen, fluorine or chlorine; or*
- (ii) *the substance contains oxygen, fluorine or chlorine and these elements are chemically bonded only to carbon or hydrogen.*

For inorganic solids, assessment of oxidising properties does not have to be done if the substance does not contain any oxygen or halogen atoms, according to Section 2.14.4.2 of Annex I to the CLP Regulation.

The sentence quoted referred to above from REACH Annex VII, which allows waiving of further testing, namely “[...] if the preliminary test clearly indicates that the test substance has oxidising properties” is relevant only when using the A.17 test method of Regulation (EC) 440/2008, which is not the preferred test method since it belongs to the DSD classification system. The O.1 test method used for classification according to the CLP Regulation does not include any preliminary test.

Waiving possibilities according to Annex XI to REACH

USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS REFERRED TO IN ARTICLE 13 (3) OF REACH

The O.1 test method of the UN Manual of Tests and Criteria is also used for classification according to the UN Model Regulations on the Transport of Dangerous Goods, and consequently also in the various regulations on transport of dangerous goods e.g. ADR and RID. A solid that has been classified as belonging to Division 5.1 according to the regulations on transport of dangerous goods on the basis of results from the O.1 test method, is an Oxidising Solid according to the criteria of the CLP Regulation.

WEIGHT OF EVIDENCE

For the determination of the oxidising solids, weight of evidence is not possible.

(Q)SAR

At the time of writing, no reliable (Q)SAR-methods exist for sufficiently accurate predictions of oxidising properties. As explained above, however, assessment of the chemical structure may be used to exclude oxidising behaviour of a substance. Possibly, this relation could be exploited in the development of future (Q)SPR-methods.

GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH

At present grouping and read across are not applicable.

1 TESTING IS TECHNICALLY NOT POSSIBLE

2 Some substances may decompose upon heating. Substances may occasionally react with cellulose
3 in other ways than through oxidation of the cellulose.

4 Further waiving possibilities

5 Not foreseen.

6 Impurities; uncertainties

7 The O.1 test method is (currently) performed using the unaided eye as measuring instrument. Only
8 by expert judgement and thorough experience can the result of the test be correctly judged, and
9 even then uncertainties may arise.

10 Minor impurities will usually not influence the test, unless they are very strong oxidisers. Expert
11 judgement should be used to determine whether impurities may have an effect.

12 A few substances may show other reactions than pure oxidation of the cellulose, or may
13 decompose. If this is suspected, expert judgement should be sought.

14 How to conclude on the DSD classification

15 Any substance classified as an Oxidising Solid according to the CLP Regulation criteria should
16 normally be classified with risk phrase R8 or R9 according to the DSD. The DSD-criteria for
17 classification with risk phrase R9 are not very precise, but if the CLP Regulation classification is
18 Category 1, the substance should be classified with risk phrase R9 if the reaction with cellulose is
19 violent.

20 Endpoints specific information in the registration dossier/in IUCLID**21 Material and methods**

- 22 • description of the apparatus and dimensions or reference to the standard or the test method
23 applied;
24 • particle size and distribution.
25

26 Results and discussion**27 If the O.1 test method was used:**

- 28 • indicate if a vigorous reaction was observed;
29 • indicate the maximum burning time for the test mixture;
30 • indicate the maximum burning time for the reference mixtures;
31 • interpretation of results, including any relevant special observations;
32 • estimated accuracy of the result (including bias and precision).
33
34

35 If A.17 test method was used:

- 36 • indicate if in the preliminary test, a vigorous reaction was observed;
37 • indicate the maximum burning rate for the test mixture;
38 • indicate the maximum burning rate for the reference mixture;
39 • interpretation of results, including any relevant special observations;
40 • estimated accuracy of the result (including bias and precision).
41

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on oxidising properties can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.15	VII 7.13	Oxidising properties	E.4.16	3.13

Further information / references

The ECHA *Guidance on the Application of the CLP Criteria* gives in Chapter 2.13 detailed information on the oxidising property, the CLP-classification, the O.1-test method and the relation to the DSD and the transport of dangerous goods regulations.

R.7.1.14 GRANULOMETRY

R.7.1.14.1 Type of property

Granulometry is not a specific physico-chemical property of a substance. The original particle size distribution is highly dependent on the industrial processing methods used and can also be affected by subsequent environmental or human transformations. Particle size is usually measured in micrometers (= 10^{-6} m; μm ; “microns”).

Granulometry is of considerable importance for the toxic properties of a substance as it influences aspects such as:

- the route of exposure of humans and toxicity by inhalation;
- the choice of route of administration for animal testing;
- the efficiency of uptake in an organism;
- the distribution in the environment.

In general all powder materials will have a range of particle sizes (particle size distribution), a presentation of the particle size distribution (e.g. using a histogram of the particle size vs. mass, number of particles, etc.) is necessary to interpret the data.

For inhalation exposure it is well known that the human toxicity will be related with the place of deposition into the respiratory tract. The deposition mainly depends on the properties of the particle (size, shape, density etc) that are commonly taken into account considering the aerodynamic diameter of the particle (see definition below). Thus, the general approach has been to use mass fractions (e.g. health related fractions as defined by EN 481 or the EPA PM Fractions). For instance, in Europe, from the publication of the EN 481 the OELs for powder materials have been defined for one or several fractions (inhalable, thoracic or respirable).

The CEN document, EN 481 “Workplace Atmospheres – size fraction definitions for measurement of airborne particles” (CEN 1993) provides definitions of the inhalable, thoracic and respirable size fractions, and target specifications (conventions) for sampling instruments to measure these fractions. The current standard defines sampling conventions for particle size fractions which are to be used in assessing the possible health effects resulting from inhalation of airborne particles in the workplace. The different particle sizes defined in EN 481 are:

- inhalable fraction (the mass fraction of particles that can be inhaled by nose and mouth. Particles $>100\ \mu\text{m}$ are not included in the inhalable convention;
- thoracic fraction (the mass fraction of the inhaled particles that passes the larynx). The convention for thoracic fraction sets that 50% of the particles in air with an aerodynamic diameter of $10\ \mu\text{m}$ belong to the thoracic fraction;
- respirable fraction (the mass fraction of the inhaled particles that reaches the alveoli) The convention for thoracic fraction sets that 50% of particles with an aerodynamic diameter of $4\ \mu\text{m}$ belong to the respirable fraction.

R.7.1.14.2 Definitions

Aerodynamic diameter: the diameter of a sphere of density $1\ \text{g cm}^{-3}$ with the same terminal velocity (falling speed) due to gravitational force in calm air as the particle under the prevailing conditions of temperature, pressure and relative humidity (CEN, 1993). The aerodynamic diameter is used to compare particles of different sizes, shapes and densities and it is a useful parameter to predict where in the respiratory tract such particles may be deposited. It is used in contrast to “optical”, “measured” or “geometric” diameters which are representations of actual diameters which in themselves cannot be related with the deposition within the respiratory tract.

Particle diffusion diameter: for particles of aerodynamic diameter less than $0.5\ \mu\text{m}$, the particle diffusion diameter should be used instead of the particle aerodynamic diameter. For diffusion, the appropriate *equivalent diameter* is the diffusion (mobility) diameter. This is defined as the diameter of a sphere with the same diffusion coefficient as the particle under the prevailing conditions of temperature, pressure and relative humidity.

The parameter of interest is the effective hydrodynamic radius, or effective Stoke’s radius R_s . Particle size distribution (effective hydrodynamic radius) requires information on water insolubility. Fibre length and diameter distributions require information on the fibrous nature of the product and on stability of the fibrous shape under electron microscope conditions.

A fibre: is a water insoluble particle with an aspect ratio (length/diameter > 3) and diameter $< 100\ \mu\text{m}$. Fibres of length $< 5\ \mu\text{m}$ need not be considered.

Particle: Minute piece of matter with defined physical boundaries. (ISO/TS 27687:2008)

Agglomerate: A collection of weakly bound particles or aggregates or mixtures of the two where the resulting external surface area is similar to the sum of the surface areas of the individual components (ISO/TS 27687:2008).

Aggregate: Particle comprising strongly bonded or fused particles where the resulting external surface area may be significantly smaller than the sum of calculated surface areas of the individual components (ISO/TS 27687:2008).

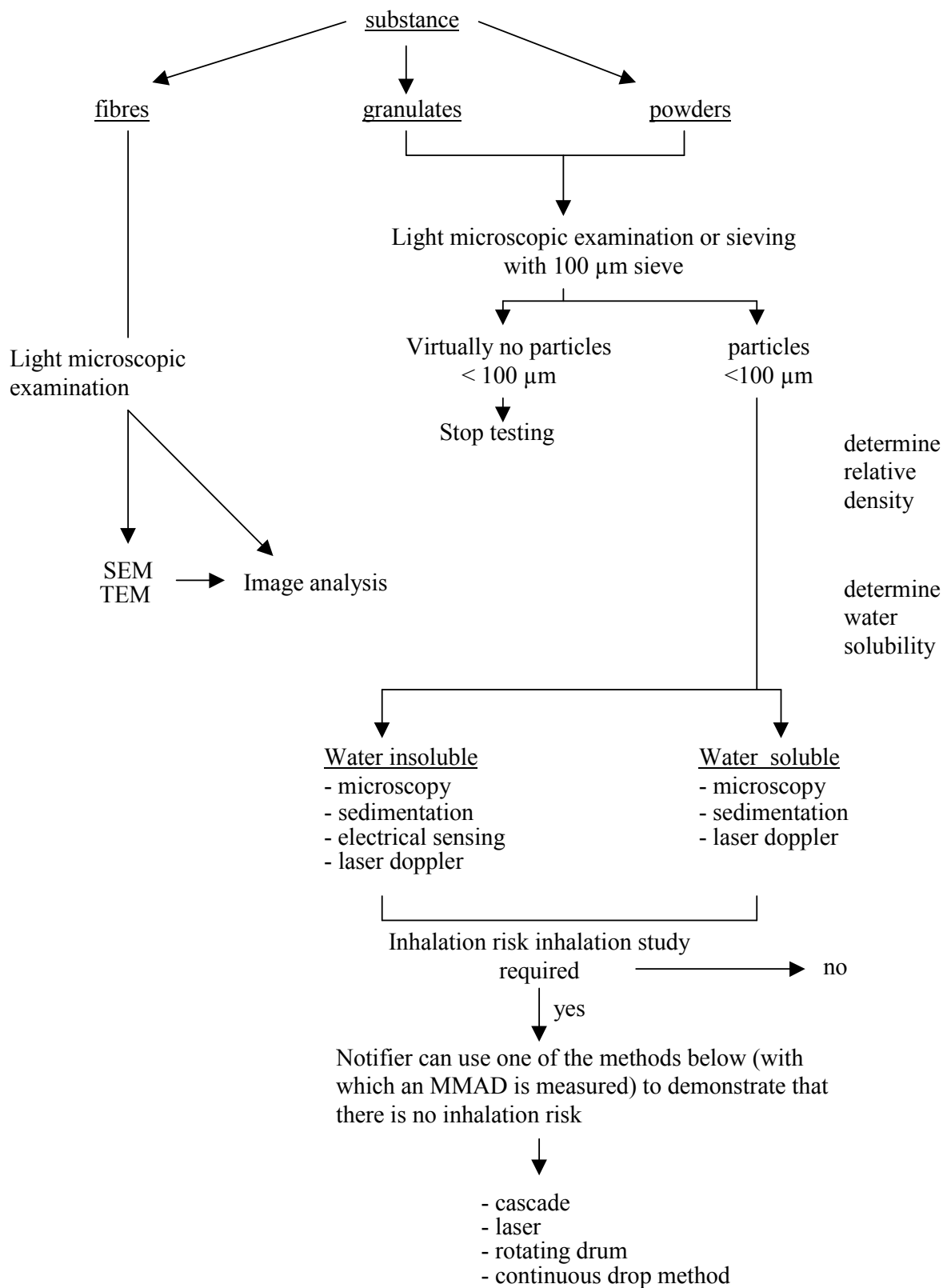
R.7.1.14.3 Test methods

Many methods are available for particle size measurements, but none of them is applicable to the entire size range (see [Table R.7.1-7](#)). Sieving, microscopic sedimentation and elutriation techniques are most commonly employed. Methods for determining particle size distribution are designed to provide information on the transportation and sedimentation of insoluble particles in water and air. An integrated testing strategy (ITS) detailing the appropriate methods for determination of particle size distribution of respirable and inhalable particles is shown in [Figure R.7.1-1](#).

Details of methods for determining particle size distribution and for fibre length and diameter distributions are outlined in OECD TG 110 and HSE Guidance document on methods for measuring particle size distribution (1996).

The particle size distribution is carried out on the material under investigation and not as airborne dust.

The measurement principle of the method used will determine what kind of diameter of the particle can be determined: for instance, optical diameter when using light scattering or aerodynamic diameter when using impactors. Methods which determine the mass median aerodynamic diameter (MMAD) need the generation of representative test atmospheres using suitable generation equipment and correct sampling techniques. They can be used in case of airborne particles (dusts, smokes, fumes), nebulised particles (wet aerosol) or dispersed particles (dry aerosol).

Figure R.7.1-1 Integrated testing strategy for granulometry

MMAD = mass median aerodynamic diameter

1

Table R.7.1-7 Methods to determine particle size distribution of a material

Method and details	Material and size range	MMAD
<p>Microscopic examination</p> <p>It is preferable to prepare samples directly in order not to influence shape and size of the particles.</p> <p>This method determines size distribution of particles.</p>	<p>Particles of all kinds</p> <p>Size range: 0.5–5000 microns (light microscope) and <0.1–10 microns (SEM/TEM)</p>	MMAD cannot be determined
<p>Sieving</p> <p>Sieving using wire-mesh sieves and perforated sheet metal sieves is not suitable to determine the distribution of particles of respirable and inhalable size since their range is only 100–10,000 microns. Micro mesh sieves (range 5–100 micron) may give better results. However, since these sieves are generally operated in combination with mechanical or ultrasonic vibration, modification of median size and form may result.</p> <p>Sieving not suitable to determine distribution of particles of respirable size, but might be suitable to determine bigger particles.</p>	<p>Dry powders/granulates</p> <p>Size range: 100–10,000 microns (wire mesh/metal sieves) and 5–100 (micromesh)</p>	MMAD cannot be determined
<p>Sedimentation (gravitational settling)</p> <p>Method is based on gravitational settling of particles in liquid and the effective hydrodynamic radius is determined. Effective hydrodynamic radius distribution should be measured 3x with no two values differing by >20%. Requires sufficient numbers of radius intervals be used to resolve the radius distribution curve. Binary or ternary mixtures of latex spheres (2–100 microns) are recommended as calibration material.</p> <p>Method might be suitable to determine the distribution of particles of respirable and inhalable size.</p>	<p>Dry powders/granulates</p> <p>Size range: 2–200 microns</p>	MMAD cannot be determined
<p>Electrical Sensing Zone (e.g. Coulter) method</p> <p>Samples are suspended in an electrolytic solution. As the particle is drawn through an aperture, the change in conductance gives a measure of particle size. The important</p>	<p>Dry powders/granulates (non-conducting)</p> <p>Size range: 1–1000 microns</p>	MMAD cannot be determined

<p>parameter is the settling velocity in the liquid phase, which depends on both density and diameter. Particles having a density of several g/cm³ can be determined.</p> <p>Applicable to particles that are complete electrical isolators in the fluid. Difference in density between particles and fluid must not be too large.</p> <p>Method might be suitable to determine the distribution of particles of respirable and inhalable size</p>		
<p>Phase Doppler Anemometry</p> <p>Expensive technique. Particle size distribution can be measured either in air or in liquid. The method presupposes that the particles are spherical with known refractive index.</p> <p>Method might be suitable to determine the distribution of particles of respirable and inhalable size</p>	<p>Dry powders/granulates</p> <p>Size range: 0.5-80 microns (in air); 0.5-1000 microns (in liquid)</p>	<p>MMAD cannot be determined</p>
<p>Determination of fibre length and diameter distributions</p> <p>Light microscopy used to examine likelihood of fibres present by comparing similarities to known fibrous or fibre releasing substances or other data. Extreme care required during sample preparation to avoid fibre breaking and clumping. Care should also be taken to avoid contamination by airborne fibres. Samples might be prepared by (a) producing suspensions in water by gentle hand agitation or vortex mixing or (b) transfer of dry material onto copper tape either directly or by spraying of the dry fibres by use of atomiser or pipette.</p> <p>Length and diameter distributions should be measured independently at least twice and at least 70 fibres counted. No two values in a given histogram interval should differ by > 50% or 3 fibres, whichever is larger. The presence of long thin fibres would indicate a need for further, more precise measurements.</p>	<p>Fibrous products</p> <p>Size range: diameters as small as 0.1 micron and as large as 100 micron and lengths as small as 5 micron and as large as 300 micron</p>	

1

2 It is advantageous to have accurate information about the propensity of materials to produce
3 airborne dust (the *dustiness* of the material). No single method of dustiness testing is likely to

1 represent and reproduce the various types of processing and handling used in industry. The
2 measurement of dustiness depends on the test apparatus used, the properties of the dust and various
3 environmental variables (i.e the dustiness is not a measurement of the “dust as it is”) . There are a
4 number of methods for measuring the dustiness of bulk materials, based on the health related
5 aerosol fractions defined in EN 481. Two methods (the rotating drum method and the continuous
6 drop method) are detailed in EN 15051 “Workplace atmospheres – Measurement of the dustiness of
7 bulk materials – Requirements and reference test methods” (CEN, 2006).

8 Dustiness is a relative term (derived from the amount of dust emitted during a standard test
9 procedure). This is dependent on the method chosen, the condition and properties of the tested bulk
10 material, and various environmental variables in which the tests are carried out. Thus, the two
11 methods in EN 15051 may provide different results (the methods are intended to simulate handling
12 processes) The standard is currently under revision (draft of European standard available) and the
13 final publication is expected for 2013. The standard has been divided in 3 parts (a general part and
14 one part for each of the methods). The methods (Table R.7.1-8) as described in the standard are
15 used to determine dustiness in terms of the health related fractions defined by EN 481. Further
16 analyse (e.g. analysing the contents on the dust collection stages) can be used to obtain the particle
17 sizedistribution. These methods require the generation of representative test atmospheres using
18 suitable generation equipment and correct sampling techniques.
19

1

Table R.7.1-8 Methods to generate/sample airborne dispersed or nebulised particles

Method and details	Material and size range	MMAD
<p>Cascade impaction</p> <p>Cascade impactors can be used to obtain the size distribution of an aerosol (i.e in this context a dust cloud). Air samples are drawn through a device which consists of several stages on which particles are deposited on an impactation substrate. Particles will impact on a certain stage depending on their aerodynamic diameter . The cut-off size can be calculated from the jet velocities at each stage by weighing each stage before and after sampling and the MMAD derived from these calculations.</p> <p>This is a well established technique to measure the size distribution of particles (allowing calculating any mass fraction). Some models are specifically designed to give the 3 health related fractions defined by the EN 481.</p>	<p>Particles in an aerosol</p> <p>Size range: 0.1-20 and 0.5-80 microns</p>	<p>MMAD can be determined via an appropriate coupled analytical technique.</p>
<p>Laser scattering/diffraction</p> <p>In general, the scattering of the incident light gives distinct pattern which are measured by a detector. This technique is particle property dependent – i.e. material has unique scattering and diffraction properties which are also particle size dependent. It is important to calibrate the instrument with similar material (of the same size range as the material to be measured). Laser scattering techniques are suitable for geometric particles, viz spheres, cubes and monocrystals. Particle size will be established optically. The MMAD can be calculated by means of a calculation correction.</p> <p>Further information about corrections and limitations of the</p>	<p>Particles of all kind</p> <p>Size range: 0.1-100 microns</p>	<p>MMAD can be determined.</p>

methods can be found in CEN/TR 16013-1 and CEN/TR 16013-2.		
<p>Rotating drum method (prEN 15051-2)</p> <p>This method is based on size selective sampling of an airborne dust cloud produced by the repeated lifting and dropping of a material in a rotating drum. Air drawn through the drum passes through a specially designed outlet and a 3-stage fractionating system consisting of two porous polyurethane foams and a membrane filter. The mass of dust collected on each collection stage is determined gravimetrically to give a direct measure of the biologically relevant size fractions. This method simulates a wide range of material handling processes in industry and determines the biologically relevant size functions of a material in the airborne state. This method is suitable to determine the respirable thoracic or inhalable fractions.</p>	<p>Dry powders/granulates/friable products</p> <p>Size range: 0.5-10,000 microns</p>	MMAD cannot be determined.
<p>Continuous drop method (prEN 15051-3)</p> <p>This method is based on the size selective sampling of an airborne dust cloud produced by the continuous single dropping of material in a slow vertical air current. The dust released by dropping material is conducted by the airflow to a sampling section where it is separated into the inhalable and respirable fractions. This method is suitable to determine the respirable and inhalable fractions.</p>	<p>Dry powders/granulates/friable products</p> <p>Size range: 0.5-10,000 microns</p>	MMAD can be determined.

Table R.7.1-9 Methods that measure inhalable fractions only or that give no detailed distributions

Method and details	Material and size range	MMAD
<p>Elutriation</p> <p>Particles are drawn out on a column at varying velocity. The velocity is used to calculate particle size and the weight of the remaining sample at a particular velocity is used to calculate the distribution. The method is limited to particles >15 microns. The method is not suitable to determine the distribution of particles of respirable size, but might be suitable to determine the distribution of particles of inhalable size</p>	<p>Dry powders/granulates</p> <p>Size range: 15-115 microns</p>	MMAD cannot be determined.
<p>Air jet sieve</p> <p>Air is aspirated through a weighted sample on a fine sieve and the weight loss measured. The method is capable of estimating the non-floatable fraction of the material under investigation. Aggregation of the particles will result in unreliable values. In addition, since the lower detection limit is only 10 micron, this method is not suitable to determine the distribution of particles of respirable size. The method is not suitable to determine the distribution of particles of the respirable fraction, but might be suitable to determine the distribution of particles between 10 and 10,000 microns..</p>	<p>Particles of all kind</p> <p>Size range: 10-10,000 microns</p>	MMAD cannot be determined.
<p>Cyclons</p> <p>The use of a cyclone is a simple approach to determining whether respirable and/or inhalable particles are present in the test atmospheres by constructing the cyclone cut off points at 4.25 and 100 microns. By measuring the weight of particles which pass</p>	<p>Particles of all kind</p> <p>Size range: 0.1-200 microns</p>	MMAD cannot be determined.

through the cyclone it can be decided whether more sophisticated methods have to be applied to determine the size distribution of the particles smaller than 10 micron. This method is suitable to determine the respirable, thoracic or inhalable fraction.		
---	--	--

1

2 **R.7.1.14.4 Adaptation of the standard testing regime**

3 Waiving possibilities according to column 2 of Annex VII to REACH

4 The study does not need to be conducted if the substance is marketed or used in a non solid or
5 granual form.

6 Waiving possibilities according to Annex XI to REACH

7 **Use of existing data: Data on physical-chemical properties from experiments not carried out** 8 **according to GLP or the test methods referred to in Article 13 (3) of REACH**

9 As the granulometry of a substance is highly dependent on the industrial processing methods and
10 possibly also on handling of the material, any published data on granulometry will be pertinent only
11 to the particular sample or process.

12 There are a number of web sites and electronic databases that include compilations of and
13 evaluations of data on particle properties. However, there appear to be a limited number of
14 reference books that provide particle size data.

15 The equivalence of the various national and international standard methods for particle size
16 distribution has not been tested and is not known.

17 **Weight of evidence**

18 In some situations where data is available from multiple sources (e.g. information on particle size
19 distribution of different batches, or information from different methods), a weight of evidence
20 approach may be used.

21 **(Q)SAR**

22 There are no QSPR/(Q)SAR tools available for predicting particle size and the data will therefore
23 need to be experimentally determined. Application of (Q)SAR is not possible.

24 **Grouping of substances and read-across approach**

25 At present grouping and read across are not applicable.

1 **Testing is technically not possible**

2 In this case testing should always be possible for solids or granular substances.

3 Further waiving possibilities

4 Not foreseen.

5 **R.7.1.14.5 Impurities; uncertainties**

6 There is a particular problem in relation to sedimentation and Coulter counter measurements. The
7 effect of impurities on particle shape should be considered when measuring fibre length and
8 diameter distributions.

9 The small quantities used as samples must be representative of product batches comprising many
10 kilograms; therefore sampling and sample handling require great care.

11 Great care should also be taken due to the fact that non-conducting particles in a non-conducting
12 liquid may be electrically charged resulting in non-representative settling of particles of a certain
13 size. In addition, in the process of particle size distribution determination, it is very important to
14 take the electrostatic charge of the particles into account. Electrostatically charged particles behave
15 differently and may influence sampling.

16 It is useful to distinguish between aggregates and agglomerates. While an aggregate is held together
17 by strong forces and may be considered to be permanent, agglomerates are held together with weak
18 forces and may break up under certain circumstances. As small particles often form agglomerates,
19 sample pre-treatment (e.g. the addition of dispersing agents, agitation or low-level ultrasonic
20 treatment) may be required before the primary particle size can be determined. However, great care
21 must be taken to avoid changing the particle size distribution.

22 **R.7.1.14.6 Endpoint specific information in the registration dossier / in IUCLID**

23 **Material and methods**

- 24 • sample preparation, such as any sonication, grinding, or addition of dispersion agents (if any)
25 • if a suspending medium is used (e.g. sedimentation test): indicate type of medium, temperature
26 pH, and concentration
27 • The type of method used
28

29 **Results and discussion**

- 30
31 • in the particle size field: mean and standard deviation
32 • in the particle size distribution at different passages field: size and
33 distribution
34 • shape of the particles
35 • for fibres: indicate both length and diameter of fibres
36 • estimate value for the accuracy of the result (including bias and precision)
37 • results for a (standard) reference material
38

39 If there are any deviations from the guideline method used or other special considerations then these
40 should be reported. In cases where there is more than one source of data, the endpoint summary
41 under results and discussion should provide a justification for the selection of the key study chapter.
42

1 **Reference to other ECHA Guidance Documents**

2 Further detailed guidance on particle size distribution (Granulometry) can be found in the following
3 chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.5	VII 7.14	Particle size distribution (Granulometry)	E.4.6	3.4

4 **R.7.1.14.7 Further information / references**

CEN 1993	EN 481: Workplace atmospheres. Size fraction definitions for measurement of airborne particles
CEN 2006	EN 15051: Workplace atmospheres. Measurement of the dustiness of bulk materials – Requirements and reference test methods
HSE 1996	The Notification of New Substances (NONS): Guidance document on methods for measuring particle size distribution
OECD TG 110	Test No. 110: Particle size distribution/fibre length and diameter distributions
prEN 15051-1 rev	Workplace exposure - Measurement of dustiness of bulk materials - Part 1: Requirements and choice of test methods
prEN 15051-2	Workplace exposure - Measurement of the dustiness of bulk materials - Part 2: Rotating drum method
prEN 15051-3	Workplace exposure - Measurement of the dustiness of bulk materials - Part 3: Continuous drop method
(ISO/TS 27687:2008)	Nanotechnologies-Terminology and definitions for nano-objects- Nanoparticle, nanofibre, and nanoplate
CEN/TR 16013-1:2010	Workplace exposure. Guide for the use of direct-reading instruments for aerosol monitoring. Choice of monitor for specific applications
CEN/TR 16013-2:2010	Workplace exposure. Guide for the use of direct-reading instruments for aerosol monitoring. Evaluation of airborne particle concentrations using optical particle counters

R.7.1.15 ADSORPTION/DESORPTION

R.7.1.15.1 Type of property

Adsorption/desorption is not a specific physico-chemical property of a substance. This property indicates the binding capacity (or *stickiness*) of a substance to solid surfaces, and so is essential for understanding environmental partitioning behaviour.

Information on adsorption/desorption is an essential input to environmental exposure models, because:

- adsorption to suspended matter can be an important physical elimination process from water in sewage treatment plants (STPs). This in turn may mean that sewage sludge, if spread to land, is a major source of the substance in soil;
- adsorption to suspended matter in receiving waters affects both the concentration in surface water and the concentration in sediment;
- desorption of a substance from soil directly influences its mobility and potential to reach surface or groundwaters.

Consequently, information on adsorption/desorption is also an important factor in test strategies for assessing toxicity to sediment- or soil-dwelling organisms.

Substances that adsorb strongly to biological surfaces (e.g., gills, skin, etc.) may lead to toxic effects in higher organisms after biomagnification.

The information is also relevant for assessing environmental persistence. For example: Degradation rates in sediment and soil are also assumed to be reduced by default if a substance is highly sorptive (since it is less bioavailable to microorganisms). This may lead to consideration of soil/sediment simulation testing in some cases.

Finally, there may be practical implications for test performance: Substances that adsorb strongly to surfaces can be difficult to test in aquatic systems.

R.7.1.15.2 Definition

Adsorption is caused by temporary (reversible) or permanent bonding between the substance and a surface (e.g. due to Van der Waals interactions, hydrogen bonding to hydroxyl groups, ionic interactions, covalent bonding, etc.). For more information please check the OECD guidances listed in the sub-chapter on Further information/ references (OECD 2000a, OECD 2000b, OECD 2001, OECD 2002).

R.7.1.15.3 Test method(s)

The adsorption of a substance to sewage sludge, sediment and/or soil can be measured or estimated using a variety of methods, which are tabulated in Table R.7.1-10 in order of increasing complexity. The dissociation constant (if appropriate) should be known before testing. Information on vapour pressure, solubility in water and organic solvents, octanol-water partition coefficient and stability/degradability is also useful.

Table R.7.1-10 Methods for the measurement of adsorption

Method and Description	Applicability/Notes
<p>Adsorption control within an inherent biodegradability test</p> <p>Estimate of the extent of adsorption to STP sludge made from the elimination level in a Zahn-Wellens inherent biodegradation test. (e.g. OECD TG 302B). 3-hour value recommended. Values beyond 24 hours not normally used. Where data are not available for adsorption up to 24 hours, data from time scales beyond this can only be used if adsorption is the only removal mechanism, with an upper limit of 7 days.</p>	<p>Highly adsorptive substances that are water soluble</p>
<p>HPLC method: OECD TG 121; EU C.19: Estimation of the Adsorption Coefficient (K_{oc}) on Soil and on Sewage Sludge using High Performance Liquid Chromatography (HPLC) (Original Guideline, adopted 22nd January 2001)</p> <p>Calibration with reference substances (preferably structurally related to the test substance) of known K_{oc} allows the K_{oc} of the test substance to be estimated. Test substance K_{oc} value should lie within the calibration range of the reference substances.</p>	<p>Measurement of $\log K_{oc}$ in the range 1.5-5.0.</p> <p>Validated for several chemical types, see test guideline for details.</p> <p>Poorly soluble and volatile substances as well as mixtures.</p> <p>Ionisable substances: test both ionised and unionised forms in appropriate buffer solutions where at least 10 % of the test compound will be dissociated within pH 5.5 to 7.5</p> <p>May not be suitable for: substances that react with the column, solvent or other test system components; surface active substances; substances that interact in a specific way with inorganic soil components such as clay minerals; inorganic compounds; moderate to strong acids and bases.</p>
<p>Batch test of adsorption of substances on activated sludge (International Standard 18749)</p> <p>Screening method to determine the degree of adsorption of substances on activated or primary sludge in sewage treatment plants (ISO, 2004). The method does not differentiate between adsorption and other elimination methods (such as complex formation, flocculation, precipitation, sedimentation or biodegradation).</p>	<p>Suitable for substances that:</p> <ul style="list-style-type: none"> are water soluble, or allow for stable suspensions/dispersions/emulsions, are not significantly removed by abiotic processes (e.g. stripping/foaming), do not de-flocculate activated sludge, are not readily biodegradable, and have a sufficiently sensitive analytical method.
<p>Sediment and soil adsorption/desorption isotherm (OPPTS 835.1220)</p> <p>Screening method according to US-EPA guideline (OPPTS, 1996) using three soil types.</p>	
<p>Batch equilibrium method (OECD TG 106; EU C.18: Absorption – Desorption Using a Batch Equilibrium Method (Updated Guideline, adopted 21st January 2000)</p> <p>Test uses a range of actual soils and so represents a more realistic scenario than the HPLC (OECD 112) method.</p>	<p>Used for substances with K_{oc} values that cannot be reliably determined using other techniques (e.g. surfactants).</p> <p>Requires a quantitative analytical method for the substance, reliable over the range of test concentrations.</p> <p>For ionisable substances, soil types should cover a wide range of pH.</p> <p>Adjustments for poorly soluble substances given in the test guideline.</p>
<p>OECD TG 312: Leaching in Soil Columns (Original Guideline, adopted 13th April 2004)</p> <p>K_d values can be derived from column leaching studies.</p>	<p>Appropriate study design to estimate K_d values particularly for unstable test substances that degrade significantly during the equilibrium time of 'shake flask' sorption studies</p>

Simulation tests and direct field measurement: including OECD guidance document no. 22 (OECD, 2000b). Monolith lysimeters can be used to study the fate and behaviour of substances in an undisturbed soil profile under outdoor conditions. They allow for monitoring of the volume of leaching/drainage water as well as the concentrations of a substance and its transformation products. They are mainly used in pesticide studies. Field leaching studies can also be carried out where hydrodynamically isolated soil layers are analysed *in situ*. Although such studies are the most realistic, their reproducibility and representativity may be limited (e.g. due to the effects of large-scale soil structure, weather events, the soil conditions at the time of application, etc.). Since data from these methods are unlikely to be encountered for the vast majority of industrial substances, they are not considered further here. Further information can be found in guidance for pesticide registration.

1

2 **R.7.1.15.4 Adaptation of the standard testing regime**

3 Waiving possibilities according to column 2 of Annex VII to REACH

4 Screening information on adsorption (and desorption) is required for substances manufactured or
 5 imported in quantities of 10 t/y or more. Depending on the results, further information (for example,
 6 a test) may be required for substances manufactured or imported in quantities of 100 t/y or more.

7 Column 2 of REACH Annexes VIII and IX provides two exemptions.

8 *A study does not need to be conducted if:*

- 9 - *based on the physicochemical properties the substance can be expected to have a low potential*
 10 *for adsorption (e.g. the substance has a low octanol water partition coefficient), or*
- 11 - *the substance and its relevant degradation products decompose rapidly.*

12 Or in other words:

- 13 - the substance can be expected to have a low potential for adsorption based on its physico-
 14 chemical properties (e.g. low octanol-water partition coefficient); or
- 15 - the substance and its relevant degradation products decompose rapidly. Therefore note that if a
 16 substance hydrolyses then it might be more appropriate to also determine the degree of
 17 adsorption of the hydrolysis products.

18 In practice a cut off value for log K_{ow} of 3 can be applied for adsorption potential. However, caution
 19 should be exercised in this criterion's use as substances that are water soluble and have a low
 20 octanol-water partition coefficient do not necessarily always have a low adsorption potential. A
 21 *measured* adsorption coefficient is usually needed for ionising substances, since it is important to
 22 have information on pH-dependence (cationic substances in particular generally adsorb strongly).
 23 Similarly, measured values will normally be needed for surface active substances (e.g. surfactants),
 24 because K_{ow} values (predicted or measured) are likely to be poor predictors of adsorption for these
 25 types of substance. For ionisable substances, partition coefficients should also be corrected
 26 according to the pH of the environment being assessed (see Annex 2). For complex mixtures (e.g.
 27 UVCBs) a single value of K_{oc} will not be definitive. In such cases a range of values or a
 28 representative value can be given, depending on the substance.

Waiving possibilities according to Annex XI to REACH

USE OF EXISTING DATA: DATA ON PHYSICAL-CHEMICAL PROPERTIES FROM EXPERIMENTS NOT CARRIED OUT ACCORDING TO GLP OR THE TEST METHODS REFERRED TO IN ARTICLE 13 (3) OF REACH

For all organic substances manufactured or supplied in quantities of 10 t/y or more, the K_{oc} should be estimated using read-across or QSPR methods as a first step. If the property is likely to be a significant determinant in the calculation of risk (e.g. following a sensitivity analysis), then a test should be conducted to provide a more reliable value for substances manufactured or supplied in quantities of 100 t/y or more. In general, confirmatory testing would not be expected for non-ionising substances with a log K_{ow} value below 3, or for substances that degrade rapidly (in which case the degradation products may be more relevant). The HPLC method may be used as a first step in testing, with the batch equilibrium method being considered only if more definitive data become necessary for the Chemical Safety Assessment. Column leaching studies might be an option under some circumstances (e.g. for unstable test substances that degrade significantly during the equilibrium time of *shake flask* sorption studies).

If estimation methods are not appropriate (e.g. because the substance is a surfactant or ionisable at environmentally-relevant pH), then a batch equilibrium test may need to be considered at the 10 t/y band, and would be essential at the 100 t/y band.

WEIGHT OF EVIDENCE

For the determination of adsorption/desorption, weight of evidence is not possible.

(Q)SAR

For all organic substances manufactured or supplied in quantities of 10 t/y or more, the K_{oc} should be estimated using read-across or QSPR methods as a first step. If the property is likely to be a significant determinant in the calculation of risk (e.g. following a sensitivity analysis), then a test should be conducted to provide a more reliable value for substances manufactured or supplied in quantities of 100 t/y or more.

Soil sorption (K_{oc}) of organic non-ionic substances can often be estimated from their octanol-water partition coefficient (K_{ow}), as well as from other properties such as aqueous solubility. Such methods, including QSPR, are useful in the first instance to indicate the qualitative/quantitative adsorption coefficient of a substance. In some instances an estimated value may be sufficient for this endpoint. In all such cases the estimated method must be proven to be valid for the type of substance considered (see the general guidance for use and applicability of QSPR), and if possible a sensitivity analysis should be conducted with values generated from different models. Using a range of values in the CSA will help to highlight if the adsorption coefficient is an important factor for environmental behaviour of the substance. In general an estimated value will be sufficient if it is indicated that the adsorption coefficient will not affect the CSA, i.e. no risk is identified for the sediment/soil compartments. Estimated values are essential for substances for which experimental measurement is not feasible i.e. for *difficult substances*. Estimated values are also useful for comparing screening tests [e.g. HPLC method (OECD 121; EC C19)]. A number of reviews of K_{oc} prediction have been published recently (Lyman 1990, Reinhard & Drefahl 1999, Doucette 2000, Delle Site 2001, Doucette 2003, Dearden 2004). That of Doucette (2000) contains a number of worked examples of the estimation of log K_{oc} values.

1 Gerstl (1990) found a good correlation with $\log K_{ow}$ for a large diverse data set:

2
$$\log K_{oc} = 0.679 \log K_{ow} + 0.094$$

3
$$n = 419 \quad r^2 = 0.831 \quad s \text{ not given}$$

4 Briggs (1981) found a good correlation for a large set of pesticides:

5
$$\log K_{om} = 0.53 \log K_{ow} + 0.64$$

6
$$n = 105 \quad r^2 = 0.90 \quad s \text{ not given}$$

7 Note that the soil sorption term here is K_{om} , where *om* stands for *organic matter*. The relationship
8 between K_{oc} and K_{om} is: $\log K_{oc} = \log K_{om} + 0.2365$ (Nendza 1998).

9 Hence from the two correlations above an estimate of K_{oc} or K_{om} can readily be obtained.

10 The Abraham descriptors have been used (1999) to model K_{oc} values of a large diverse data set:

11
$$\log K_{oc} = 0.74 R - 0.31 \Sigma\alpha^H - 2.27 \Sigma\beta^O + 2.09 V_X + 0.21$$

12
$$n = 131 \quad r^2 = 0.955 \quad s = 0.245$$

13 where R = excess molar refractivity (a measure of polarisability), $\Sigma\alpha^H$ = hydrogen bond donor
14 ability, $\Sigma\beta^O$ = hydrogen bond acceptor ability of oxygen, and V_X = McGowan molecular volume.
15 The descriptors are approximately auto-scaled, so that the magnitude of each coefficient is an
16 indication of the relative contribution of each descriptor to soil sorption. Hence hydrogen bond
17 acceptor ability and molecular size appear to be the most important factors controlling soil sorption.

18 **GROUPING OF SUBSTANCES AND READ-ACROSS APPROACH**

19 Read-across and/or QSPR prediction for K_{oc} are important predictive tools and should be the first
20 method used to predict K_{oc} if reliable measured data do not exist and the model is valid for the
21 substance. However if these options do not give meaningful and valid information or if K_{oc} is an
22 important factor in the CSA (i.e. risks are indicated for sediment/soil compartments based on a
23 predicted value and $\log K_{ow}$ is >3), then an experimental value should be measured.

24 **TESTING IS TECHNICALLY NOT POSSIBLE**

25 In this case testing should always be possible. In general, partition coefficients that are measured
26 with a suitable standard method are preferred (and they are usually essential for surfactants and
27 ionic substances that dissociate at environmentally relevant pH).

28 Further waiving possibilities

29 Not foreseen. The K_{oc} is not directly relevant for environmental classification or the PBT
30 assessment. However, it is a key property for exposure assessment so the information requirement
31 should not be waived.

R.7.1.15.5 Impurities;uncertainties

Impurities can have an impact on the measurement of adsorption/desorption. Expert judgement should be used when considering whether impurities may affect the determination of the adsorption/desorption.

R.7.1.15.6 Endpoint specific information in the registration dossier/ in IUCLID

HPLC method (OECD TG 121, EU C.19)

Materials and methods

- description of the HPLC equipment and operating conditions (column, mobile phase, means of detection, temperature);
- dead time and method used for its determination;
- reference substances (identity, purity, K_{oc}, retention times) with results of at least 6 measurements with at least one of them above and one below the expected value for the test substance;
- quantities of test and reference substances introduced in the column.

Results and discussion

- average retention data and estimated d log K_{oc} value for test compound;
- all values of log K_{oc} derived from individual measurements.

Batch equilibrium method (OECD TG 106, EU C.18)

Materials and methods

- details on soil types (nature and sampling site(s), organic C, clay content and soil texture, and pH, if relevant Cation Exchange Capacity);
- information on the test substance (nominal and analytical test concentrations, stability and adsorption on the surface of the test vessel, solubilising agent if relevant (and justification for its use), radiochemical purity if relevant);
- details on test conditions (e.g. soil/solution ratio, number of replicates and controls, sterility, test temperature, and pH of the aqueous phase before and after contact with the soil);
- details on sampling (e.g. frequency, method);
- details on the analytical methods used for determination of the substance (detection limit, recovery %);

Results and discussion

- soil dry mass, total volume of aqueous phase, concentration of test substance in solution and/or soil after agitation and centrifugation, equilibration time, K_{oc}, if appropriate mass balance;
- explanations of corrections made in the calculations, if relevant (e.g. blank run);

Leaching in soil columns (OECD TG 312)

Materials and methods

- details on soil types (nature and sampling site(s), organic C, clay content and soil texture, Cation Exchange Capacity, bulk density (for disturbed soil), water holding capacity and pH;
- information on the test substance (amount of test substance and, if appropriate, reference substance applied, solubilising agent if relevant (and justification for its use), radiochemical purity if relevant);

- details on test conditions (number of replicates and controls, test temperature, amount, frequency and duration of application of artificial rain);
- details on the analytical methods used for determination of the substance (detection limit, recovery %);
- reference substance used.

Results and discussion

- Koc, tables of results expressed as concentrations and as % of applied dose for soil segments and leachates;
- mass balance, if appropriate;
- leachate volumes;
- leaching distances and, where appropriate, relative mobility factors.

Adsorption control within an inherent biodegradability test (OECD TG 302B)

Materials and methods

- details on inoculum;
- Information on the test substance (toxicity to bacteria, test concentration);
- details on test conditions (blank controls used, inoculum and test compound ratio (as DOC));
- details on sampling (frequency);
- details on the analytical methods used for determination of the DOC or COD;
- reference substance.

Results and discussion

- estimate of the extent of adsorption to STP sludge made from the elimination level in this Zahn-Wellens inherent biodegradation test, based on the 3-hour value if possible;
- values beyond 24 hours should not normally be used but where data is not available for adsorption up to 24 hours, data from time scales beyond this can only be used if adsorption is the only removal mechanism, with an upper limit of 7 days;
- if relevant results of testing of inhibition of biodegradation.

Simulation test/field measurement (OECD TG 22)

Materials and methods

- details on soil types (nature and sampling site(s); if relevant: organic C, clay content and soil texture, Cation Exchange Capacity and pH;
- details on lysimeter;
- information on the test substance (nominal and analytical test concentrations, solubilising agent if relevant (and justification for its use), radiochemical purity if relevant);
- details on test climate conditions (e.g. air temperature, solar radiation, humidity, potential evaporation or rate of artificial rainfall), soil temperature and soil moisture and duration of the study;
- details on sampling (frequency, method);
- details on the analytical methods used for determination of the test substance (detection limit, recovery %).

Results and discussion

- concentration of test substance in soil layers; Koc, if appropriate mass balance and concentrations and as % of applied dose for soil segments and leachates;
- explanations of corrections made in the calculations, if relevant (e.g. blank run).

Distribution modelling**Materials and methods**

- model name and version;
- date of the model development;
- model type description e.g. steady-state, dynamic, fugacity, Gaussian, Level I-IV, etc.;
- environmental compartments which the model covers;
- information on model segmentation and environmental properties;
- input parameters (minimum information required for assessing the partitioning and degradation behaviour):
 - vapour pressure;
 - water solubility;
 - molecular weight;
 - octanol-water partition coefficient;
 - information on ready biodegradability;
 - for inorganic substances: it is recommended to have information on the partition coefficients and possible abiotic transformation products;
- temperature effect.

Results and discussion

- key exposure routes and distribution of the substance among them.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on adsorption/desorption can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
5.4.1	VIII 9.3.1	Adsorption / desorption	E.5.5.2	4.1.4
5.4.2	/	Henry's Law constant	E.5.5.3	4.1.4
5.4.3	X 9.3.4	Distribution modelling	E.5.5.4	4.1.4
5.4.4	X 9.3.4	Other distribution data	E.5.5.5	4.1.4

R.7.1.15.7 Further information/references

- Briggs G.G. (1981) Theoretical and experimental relationships between soil adsorption, octanol-water partition coefficients, water solubilities, bioconcentration factors and the parachor. *J. Agric. Food Chem.* 29, 1050-1059.
- Dearden J.C. (2004) QSAR modelling of soil sorption. In Cronin M.T.D. and Livingstone D.J. (Eds.), *Predicting Chemical Toxicity and Fate*, CRC Press, Boca Raton, FL, pp. 357-371.
- Delle Site, A., (2001) Factors affecting sorption of organic compounds in natural sorbent/water systems and sorption coefficients for selected pollutants. *J. Phys. Chem. Ref. Data* 30, 187-439.
- Doucette W.J. (2000) Soil and sediment sorption coefficients. In Boethling R.S. and Mackay D. (Eds.), *Handbook of Property Estimation Methods for Chemicals: Environmental and Health Sciences*. Lewis, Boca Raton, FL, pp. 141-188.
- Doucette W.J. (2003) Quantitative structure-activity relationships for predicting soil/sediment sorption coefficients for organic chemicals. *Environ. Toxicol. Chem.* 22, 1771-1788
- ECETOC (1998). Technical Report No. 74: QSARs in the Assessment of the Environmental Fate and Effects of Chemicals. European Centre for Ecotoxicology and Toxicology of Chemicals. Brussels.
- EU C18 Adsorption – desorption using a batch equilibrium method.
- EU C19 Estimation of the adsorption co-efficient (K_{oc}) on soil and on sewage sludge using high performance liquid chromatography (HPLC).
- Gerstl Z. Estimation of organic chemical sorption by soils. *J. Contaminant Hydrology* (1990) 6, 357-375.
- ISO (2004). Water quality: adsorption of substances on activated sludge – batch test using specific analytical methods. International Standards Guideline 18749. First edition February 2004.
- Lyman W.J. Adsorption coefficient for soils and sediments. In Lyman W.J., Reehl W.F. and Rosenblatt D.H. (Eds.), *Handbook of Chemical Property Estimation Methods*, American Chemical Society, Washington DC, 1990, pp. 4.1-4.33.
- Mueller, M. and Kordell, W. (1996). Comparison of screening methods for the estimation of adsorption coefficients on soil. *Chemosphere* 32(12), 2493-2504.
- Nendza M. *Structure-Activity Relationships in Environmental Sciences*. Chapman & Hall, London, 1998.
- OECD (2000a). Adsorption – desorption using a batch equilibrium method. Organisation for Economic Co-operation and Development (OECD) Guideline for the testing of chemicals no 106.
- OECD (2000b) Guidance Document No. 22: Performance of Outdoor Monolith Lysimeter Studies. Organisation for Economic Co-operation and Development (OECD), Paris.
- OECD (2001). Estimation of the adsorption co-efficient (K_{oc}) on soil and on sewage sludge using high performance liquid chromatography (HPLC). Organisation for Economic Co-operation and Development (OECD) Guideline for the testing of chemicals no 121.
- OECD (2002) Guidelines for Testing of Chemicals (Draft): Leaching in Soil Columns. Organisation for Economic Co-operation and Development (OECD), Paris.

OPPTS (1996). Sediment and soil adsorption/desorption isotherm. United States Environmental Protection Agency, Office of Prevention, Pesticides and Toxic Substances Fate, Transport and Transformation Test Guideline 835.1220. Draft of April 1996.

Poole S.K. and Poole C.F. (1999) Chromatographic models for the sorption of neutral organic compounds by soil from air and water. *J. Chromatogr. A* 845, 381-400.

Reinhard M. and Drefahl A. (1999). *Handbook for Estimating Physico-chemical Properties of Organic Compounds*. Wiley, New York.

SETAC (1993). Guidance Document on Sediment Toxicity Tests and Bioassays for Freshwater and Marine Environments. From the Workshop on Sediment Toxicity Assessment at Renesse, Netherlands on 8-10 November 1993. Hill I, Mathiessen P, Heimbach F (eds). Society of Environmental Toxicology and Chemistry – Europe, Brussels.

R.7.1.16 STABILITY IN ORGANIC SOLVENTS AND IDENTITY OF RELEVANT DEGRADATION PRODUCTS

R.7.1.16.1 Type of property

The stability in organic solvents is required for substances manufactured or imported in quantities of ≥ 100 t/a only if their stability in organic solvent is considered critical (REACH Annex IX, section 7.15).

There are rare occasions when it is important to have information on the stability of a compound in an organic solvent, to ensure confidence in the test results. However, for many substances, the stability in organic solvents will not be critical and testing need not be conducted.

Examples of when stability in organic solvents could be important are:

- for certain solubility measurements (e.g. octanol–water partition coefficient);
- to check on the stability of reagent solutions, fortification standards or calibration standards;
- when a test substance is dosed as a solution in an organic solvent (e.g. ecotoxicity studies);
- when a test substance is extracted from an environmental sample, plant or animal tissue or diet matrix (arising from a variety of physicochemical property, ecotoxicity and animal toxicity studies) into an organic solvent and stored pending analytical measurement.

R.7.1.16.2 Definition

A study of the stability of a test compound in an organic solvent is normally undertaken for a specific time period to confirm whether the test compound is stable under these conditions for the duration of the storage of the organic solvent or extract containing the test substance. Often several time periods are selected to check whether there is any particular downward trend in stability over time.

The stability of the test substance at a particular time period during the study is normally expressed as a percentage of the concentration of the test substance in the solvent extract, at that time period compared with the initial starting concentration of the test substance at $t = 0$, namely:

$$\frac{C_t}{C_{t_0}} \times 100 \%$$

where C_t is the concentration of test substance in solvent extract at $t_1, t_2, t_3, \dots, t_n$; and C_{t_0} is the concentration of test substance in solvent extract at t_0 .

R.7.1.16.3 Test method(s)

A number of physical, chemical and biological processes can result in a decline in the actual concentration of a test substance in an organic solvent over time. Information on the stability of a test substance in a solvent is desirable, particularly when samples are to be stored. However, there does not appear to be any generally accepted methodology for performing such stability studies. Factors affecting the rate of degradation include rates of hydrolysis, of photolysis and of oxidation.

Typically, one or more concentrations of the test substance in the solvent are made up and analysed immediately after preparation (i.e. $t = 0$). They are then stored in appropriate vessels under the required test conditions (e.g. temperature, absence of light) and analysed, along with a freshly prepared solution of the test substance at the original test concentration(s), at regular intervals during the period of interest.

At each time of analysis, a sample is withdrawn from storage and mixed thoroughly before taking any aliquot for analysis. The analysis is carried out using the recommended method to determine whether any significant loss of the test substance has occurred during storage. It is important to analyse freshly made standards of the test substance in the organic solvent at the same time as analysing stored samples, so that any losses that may occur of the test substance during sampling, sample treatment and analysis are taken into consideration.

It is important to be able to have a check on the temperature to ensure that the temperature regime has been maintained throughout the period of the stability study.

Unlabelled reference material of suitable known purity may be used where a reliable method of analysis is available. Where an analytical method is still under development or is unlikely to be sufficiently sensitive, radio-labelled compounds should be used if available. Use of radio-labelled compounds can shorten the analysis time and help facilitate identification of any degradation products, should the test substance not be stable in the organic solvent.

Recovery or spiking experiments should normally be run. The number of spiking levels or the range of concentrations tested within a project should be left to the judgement of the analyst.

Further information should be obtained by checks on the stability of standards of the test substance in organic solvents as part of routine analytical protocols, to confirm whether the test substance is unstable under normal storage conditions.

Further tests may be necessary to identify storage conditions which minimise any degradation of the test substance not only in organic solvents, but also during the conducting of other tests, such as water solubility, surface tension and in the preparation of test media for ecotoxicity studies (OECD, 2000). Identification of the degradation product(s) will allow an assessment of whether they are likely to be more toxic than the parent material in subsequent ecotoxicity studies.

1 **R.7.1.16.4 Adaptation of the standard testing regime**

2 Waiving possibilities according to column 2 of Annex IX to REACH

3 Column 2 of REACH Annex IX provides the following specific rules for adaptation of the standard
4 information requirement for stability in organic solvents and identity of relevant degradation
5 products:

6 *The study does not need to be conducted if the substance is inorganic.*

7 Waiving possibilities according to Annex XI to REACH

8 **Use of existing data: Data on physical-chemical properties from experiments not carried out**
9 **according to GLP or the test methods referred to in Article 13 (3) of REACH**

10 Stability data of substances in organic solvents are not normally reported in standard published
11 sources of physico-chemical data. Relevant sources of basic information regarding stability and
12 storage conditions of substances are the Hazardous Substances Data Base (HSDB) and Sax's
13 'Dangerous Properties of Industrial Materials'.

14 **Weight of evidence**

15 For the determination of the stability in organic solvent and degradation products, weight of
16 evidence is not possible.

17 **(Q)SAR**

18 At present (Q)SAR is generally not applicable for determination of stability in organic solvent and
19 degradation products. Application of (Q)SAR is not possible.

20 **Grouping of substances and read-across approach**

21 At present grouping and read across are not applicable.

22 **Testing is technically not possible**

23 In this case testing should always be possible.

24 Further waiving possibilities

25 Not foreseen.

26 **R.7.1.16.5 Impurities; uncertainties**

27 Impurities can have an impact on the measurement of stability in organic solvent and degradation
28 products. Expert judgment should be used when considering whether impurities may affect the
29 determination of the stability in organic solvent and degradation products.

30 **R.7.1.16.6 Endpoint specific information in the registration dossier / in IUCLID**

31 This endpoint needs to be fulfilled on a case by case basis. As several different methods can be used
32 to document this intrinsic property, we recommend the same strategy for drafting robust study

summaries as described for the other endpoints. The general aspects described in section 2 should also be applied for this endpoint. All endpoint specific characteristics should be described in such a way that the RSS allows an independent assessment of the endpoints reliability and completeness. The objectives, methods, results and conclusions of the full study report should be reported in a transparent manner as described for all other endpoints in this practical guide.

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on stability in organic solvents can be found in:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.17	VII 7.15	Stability in organic solvents and identity of relevant degradation products	E.4.18	3.14

R.7.1.16.7 Further information / references

OECD Series on Testing and Assessment Number 23 Guidance Document on Aquatic Toxicity Testing of Difficult Substances and Mixtures, ENV/JM/MONO(2000)6 ([http://www.olis.oecd.org/olis/2000doc.nsf/LinkTo/env-jm-mono\(2000\)6](http://www.olis.oecd.org/olis/2000doc.nsf/LinkTo/env-jm-mono(2000)6))

R.7.1.17 DISSOCIATION CONSTANT

R.7.1.17.1 Type of property

Information on the dissociation constant is **supplementary data** for hazard assessment (OECD TG 112, 1981). The dissociation of a substance in water is of importance in assessing its impact upon the environment and may also influence the ADME of a substance and consequently its effects on human health. It governs the form of the substance which in turn determines its behaviour and transport. It may affect the adsorption of the substance on soils and sediments and absorption into biological cells.

The dissociation constant may also be an important factor in deciding which method or conditions should be used to determine the octanol-water partition coefficient (K_{ow}) and soil adsorption partition coefficient (K_{oc}). Slight changes in pH can considerably affect the form in which the substance is present in solution, especially if the pK_a value is within the environmentally-relevant pH range¹¹. The dissociated and non-dissociated species may have significantly different water

¹¹ Fresh surface waters have pH values in the range 4-9, whereas marine environments have a stable pH of about 8. pH normally varies between 5.5 and 7.5 for agricultural soils and sewage treatment plant tanks.

solubilities and partition coefficients. Therefore, significantly different bioavailability and toxicity may result. It is important to note that the dissolution of salts from their crystal lattice into individual ions is not intended to be covered by the endpoint dissociation constant. Therefore this section refers only to acid dissociation (pK_a).

R.7.1.17.2 Definition

Dissociation is the reversible splitting of a substance into two or more chemical species, which may be ionic (OECD TG 112, 1981). The process can be represented as:



The dissociation constant (K) for this process is expressed as the ratio of concentrations of the species on either side of the equation in water at equilibrium:

$$K = \frac{[R^+][X^-]}{[RX]}$$

Where the cation R^+ is hydrogen, the substance can be considered an acid, and so this constant becomes an acid dissociation constant (K_a).

$$K_a = \frac{[H^+][X^-]}{[HX]}$$

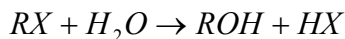
A substance can have more than one acidic (or basic¹²) group, and the dissociation constant can be derived for each dissociation step in a similar way.

The K_a is related to pH as follows (where p is $-\log_{10}$):

$$pK_a = pH - \log_{10} \left(\frac{[X^-]}{[HX]} \right)$$

In practice for a simple substance having one dissociating group, the pK_a is equivalent to the pH at which the ionised and non-ionised forms are present in equal concentration (i.e. the substance has undergone 50% dissociation).

It is important to differentiate between dissociation and hydrolysis as hydrolysis is a separate standard information requirement according to Annex VIII of the REACH regulation. Hydrolysis is defined as reaction of a substance RX with water, with the net exchange of the group X with OH at the reaction centre (OECD TG 111, 2004).



¹² Base strength is expressed as the acidity of the conjugate acid. The term pK_b was once used to express basicity so that the same scale could be used alongside acidity – care should be taken when citing older sources to check which term has been used. For consistency, dissociation of bases should preferably be expressed using the pK_a of the conjugate acid.

1 **R.7.1.17.3 Test method(s)**

2 OECD test guideline 112 (Dissociation constants in water, adopted May 1981) describes three
3 laboratory methods to determine the pK_a of a substance. The three methods are appropriate for
4 particular types of substances as described in the test guideline¹³.

5 **R.7.1.17.4 Adaptation of the standard testing regime**

6 Waiving possibilities according to column 2 of Annex IX to REACH

7 Column 2 of REACH Annex IX provides the following specific rules for adaptation of the standard
8 information requirement for dissociation constant:

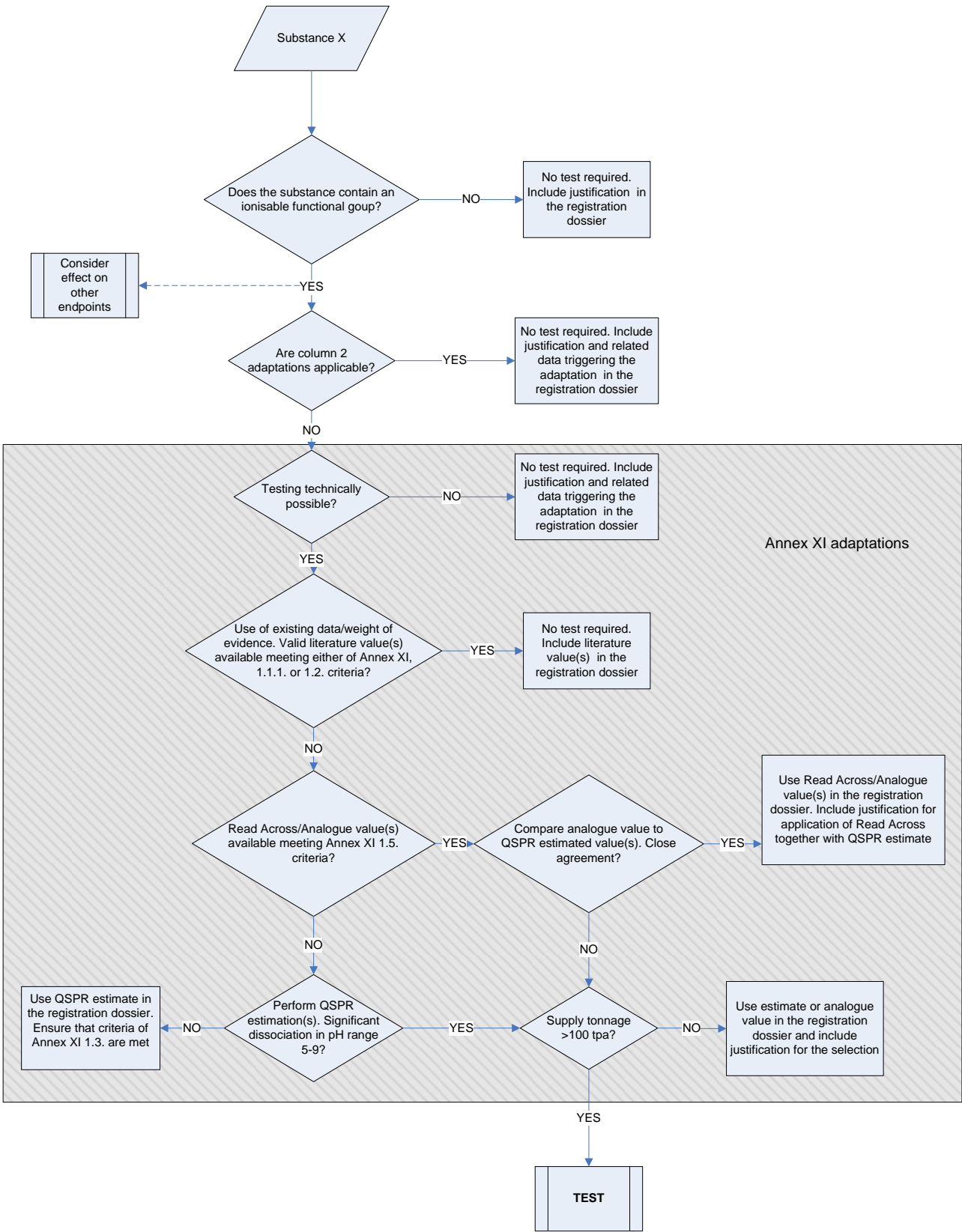
9 *A study does not need to be conducted if:*

- 10 - *the substance is hydrolytically unstable (half-life less than 12 hours) or is readily*
11 *oxidisable in water; or*
- 12 - *it is scientifically not possible to perform the test (e.g. because the analytical method is*
13 *not sensitive enough).*

14 In all cases where the above specific rules for adaptation are used to waive testing, evidence
15 demonstrating the existence of that property of the substance which triggers the adaptation rule
16 should be provided in the IUCLID dossier, e.g. if the test is not performed because the substance is
17 hydrolytically unstable (half life < 12 hours) then the dossier must contain valid data on the
18 hydrolysis clearly indicating a half life < 12 hours.

19 It is important to note that OECD TG 112 allows the use of a small amount of a water-miscible
20 solvent to aid dissolution of sparingly soluble substances. Therefore low solubility will only prevent
21 performance of the test in the context of the column 2 rules above for substances which remain
22 highly insoluble and undetectable by analytical techniques in the presence of water miscible
23 solvents.

¹³ The test method is available on the following link: http://www.oecd-ilibrary.org/environment/test-no-112-dissociation-constants-in-water_9789264069725-en



1

2 Figure xx: Integrated testing strategy for dissociation constant

1 Waiving possibilities according to Annex XI to REACH

2 **Use of existing data: Data on physical-chemical properties from experiments not carried out** 3 **according to GLP or the test methods referred to in Article 13 (3) of REACH**

4 Many literature sources for dissociation constant exist; some reference textbooks and on-line
5 sources are listed in section R.7.1.1.2. These should be searched for published, valid data. As
6 mentioned in REACH Annex XI section 1.1.1. a number of conditions need to be met before any
7 such data can be used. Namely:

- 8 - *adequacy for the purpose of classification and/or risk assessment;*
- 9 - *sufficient documentation is provided to assess the adequacy of the study; and*
- 10 - *the data are valid for the endpoint being investigated and the study is performed using*
11 *an acceptable level of quality assurance.*

12 **WEIGHT OF EVIDENCE**

13 Where data are available in the literature which do not meet the conditions listed in the Annex XI of
14 REACH section 1.1.1 a weight of evidence approach might be possible provided that data from a
15 number of distinct sources indicate a similar value for the dissociation constant which is supported
16 by one or more relevant QSPR predictions.

17 **(Q)SAR**

18 Estimated pK_a data can be generated by valid QSPR methods. In general, pK_a values that are
19 measured with a suitable method are preferred to QSPR predictions. If an estimated pK_a value
20 suggests that the substance will dissociate significantly at environmentally relevant pH, a test may
21 be required to confirm the result.

22 There have been a few attempts to model pK_a values of diverse sets of substances. Klopman and
23 Fercu (1994) used their MCASE methodology to model the pK_a values of a set of 2464 organic
24 acids, and obtained good predictions; a test set of about 600 organic acids yielded a standard error
25 of 0.5 pK_a unit. Klamt et al (2003) employed their COSMO-RS methodology to predict pK_a values
26 of 64 organic and inorganic acids, with a standard error of 0.49 pK_a unit.

27 **Grouping of substances and read-across approach**

28 For most ionisable substances supplied at greater than 100 t/y that are predicted to dissociate at
29 environmentally relevant pHs, a test will typically be required for dissociation constant. Similar
30 substances (analogues) for which measured pK_a data according to a reliable method are available
31 may be considered for read-across. Such values should be reinforced by estimated methods for pK_a
32 (e.g. the result of a QSPR prediction; see section above). In some instances it may be acceptable to
33 read-across dissociation constant from an analogue. However if there is significant variation
34 between the analogue read-across and the predicted pK_a then a test should be conducted.

Testing is technically not possible

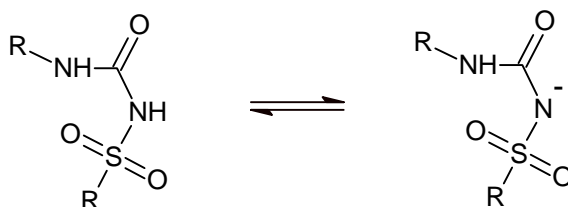
Instances where testing is technically not possible as a consequence of the properties of the substance are expected to be limited to highly reactive or unstable substances, and substances which in contact with water emit flammable gases.

Further waiving possibilities

As stated in Annex IX of REACH, when for certain endpoints, it is proposed to not provide information for other reasons than those mentioned in column 2 of that Annex or in Annex XI of REACH, this fact and the reasons must also be clearly stated. Such an approach may then be used.

No dissociating groups

If the substance cannot dissociate due to a lack of relevant functional groups, the dissociation constant is irrelevant and testing information does not need to be provided. However, ionisable groups might not always be obvious (e.g. in sulphonyl urea herbicides, which contain the function $-S(=O)_2NH.C(=O)NH-$, the acid group is $S(=O)_2NH$).



If a substance is much more soluble in water than expected, this may be an indication that dissociation has occurred.

UVCBs

For complex mixtures (e.g. UVCBs) containing ionisable components the assessment of pK_a is clearly complicated. Estimation of the representative constituent's pK_a values, if appropriate, should be considered.

R.7.1.17.5 Impurities; uncertainties

Impurities can have an impact on the measurement of dissociation constant. Expert judgement should be used when considering whether impurities may affect the determination of the dissociation constant.

The presence of multiple dissociation/equilibrium reactions can complicate determination of the dissociation constant(s). In cases where multiple dissociation reactions can take place due to the presence of numerous dissociating groups and/or the presence of tautomerisation and/or zwitterionic forms, care should be taken in the interpretation of experimental results. QSPR predictions for such substances should also be carefully analysed as the models may not account for concurrent equilibria/dissociations. Additionally QSPR predictions may not account for intramolecular hydrogen bonding effects which can have a pronounced effect on the observed dissociation constant. In some cases, formation of intramolecular hydrogen bonding depends on the cis/trans isomerism of the substance, as is the case for the isomers fumaric and maleic acid. Care should be taken when using (Q)SAR predictions for such molecules, as cis/trans isomerism is typically not taken into account.

The extent of ionisation may vary according to pH, ionic strength and/or the level of common ions in the test medium (common ion effect), and relatively small changes may significantly alter the equilibrium between dissociated and non-dissociated species.

R.7.1.17.6 Endpoint specific information in the registration dossier / in IUCLID

Knowledge of an ionisable substance's pKa is important for all substances. For substances supplied at levels below 100 tonnes per annum dissociation constant is not a testing requirement. Ideally however, a literature value, analogue value and/or QSPR prediction can be obtained and provided for such substances, especially if dissociation is relevant for interpreting the results of other physicochemical or fate and (eco)toxicological tests and for chemical safety assessment. For ionisable substances supplied at tonnages greater than 100 t/y, dissociation constant is a standard information requirement.

For substances which contain multiple ionisable functionalities, all measured macro pKa values should be reported and preferably assigned to specific micro-reactions.

With regard to study summaries of experimental data, the IUCLID dossier should contain all relevant information regarding the endpoint and as a minimum the items listed below:

Materials and methods

- type of method;
- test guideline followed.

Test Materials

- test material identity;

Results and discussion

- concentration of the substance;
- test results as pKa-value(s);
- temperature of the test medium (°C).

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on dissociation constant can be found in:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.21	IX 7.16	Dissociation constant	E.4.22	3.15

R.7.1.17.7 References on dissociation constant

- Balogh G.T., Gyarmati B., Nagy B., Molnar L. and Keseru G.M. Comparative evaluation of in silico pKa prediction tools on the Gold Standard dataset. *QSAR Comb Sci* (2009) 28:1148-1155.
- Dearden J.C., Cronin M.T.D., and Lappin D.C. A comparison of commercially available software for the prediction of pKa. *J. Pharm. Pharmacol.* (2007) 59, Suppl. 1, A-7.
- Klamt A., Eckert F., Diedenhofen M. and Beck M.E. (2003) First principles calculations of aqueous pK(a) values for organic and inorganic acids using COSMO-RS reveal an inconsistency in the slope of the pK(a) scale. *J. Phys. Chem. A* 107, 9380-9386.
- Klopman G. and Fercu D. (1994) Application of the multiple computer automated structure evaluation methodology to a quantitative structure-activity relationship study of acidity. *J. Comput. Chem.* (1994) 15, 1041-1050.
- Liao C. and Nicklaus M.C. Comparison of nine programs predicting pKa values of pharmaceutical substances. *J. Chem. Inf. Model.* (2009) 49, 2801-2812.
- Manchester J, Walkup G, Rivin O. and You Z.P. Evaluation of pKa estimation methods on 211 druglike compounds. *J Chem Inf Model* (2010) 50, 565-571.
- Meloun M. and Bordovská S. Benchmarking and validating algorithms that estimate pKa values of drugs based on their molecular structure. *Anal. Bioanal. Chem.* (2007) 389, 1267-1281.
- OECD (1981). Dissociation constants in water (titration method – spectrophotometric method – conductometric method). Organisation for Economic Co-operation and Development (OECD) Guideline for the testing of chemicals no 112.

R.7.1.18 VISCOSITY

R.7.1.18.1 Type of property

Viscosity is a property:

- needed for substance characterization;
- needed for the classification of aspiration hazard of liquids;
- which gives an indication of the penetration of the substance within soil.

R.7.1.18.2 Definition

Viscosity:

Viscosity is the (inner) resistance of a substance (gas, liquid) to a shift caused by laminar flow.

Dynamic viscosity (= dynamic viscosity coefficient) η :

Quantifies the property 'viscosity' by the quotient shear stress τ / shear rate $\dot{\gamma}$ ($\eta = \tau / \dot{\gamma}$)

Kinematic viscosity (= kinematic viscosity coefficient) ν :

is given by the quotient dynamic viscosity to density ($\nu = \eta / \rho$).

R.7.1.18.3 Test method(s)

Five different types of test methods are standardized for liquid substances:

- capillary viscometer;
- flow cup;
- rotational viscometer;
- rolling ball viscometer;
- drawn-shear viscometer.

There exist a lot of standardized determination methods with sometimes very specialised application ranges with respect to products, especially mixtures. For substances (within the scope of the REACH Regulation) the following standardised determination methods are recommended:

- Capillary viscometer:

- EN ISO 3104, EN ISO 3105, DIN 51562, BS 188, NF 60-100, ASTM D445, ASTM D4486;

- Flowcup:

- EN ISO 2431;

- Rotational viscometer:

- EN ISO 3219, DIN 53019;

- Rolling ball viscometer:

- DIN 53015;

For newtonian liquids (liquids for which the viscosity is independent of the shear stress and shear rate) any determination method may be used within the scope and applicability specifications. For non-newtonian liquids (liquids for which the viscosity depends on the shear rate) only the use of

rotational viscometers is possible. Because the viscosity is remarkably temperature dependent each determination must be accompanied by the temperature at which the measurement was made. It is recommended to use the mean of two test runs. It is also recommended to determine the viscosity at at least two different temperatures. The classification criteria for aspiration hazard refer to kinematic viscosity at 40 °C.

If explosives, pyrophorics or self-reactives are to be characterized, determination of the viscosity may not be practicable. For pyrophorics and self-reactives testing under inert gas should be considered. In any case the determination method has to be chosen carefully.

The use of the most recent update of the standard is advised; they are accessible via numerous websites, see R.7.1.1.3.

R.7.1.18.4 Adaptation of the standard testing regime

Within the REACH Regulation requirements testing of viscosity is only of interest for liquid substances.

Waiving possibilities according to column 2 of Annex IX to REACH

Column 2 of REACH Annex IX does not provide any specific rules for adaptation from column 1.

Waiving possibilities according to Annex XI to REACH

Use of existing data: Data on physical-chemical properties from experiments not carried out according to GLP or the test methods referred to in Article 13 (3) of REACH

The use of existing experimental data is possible if carried out by certified institutions.

Weight of evidence

For the determination of the viscosity, weight of evidence is not possible.

(Q)SAR

For the determination of the viscosity, (Q)SAR approaches are discouraged for the purpose of classification / risk assessment, except when the mean absolute error of the (Q)SAR is less than 5 %.

Grouping of substances and read-across approach

For the determination of the viscosity read across is not possible.

Testing is technically not possible

- if the substance is a solid;
- if liquid explosives, pyrophorics or self-reactives are to be characterized, determination of the viscosity may not be practicable (see above section Test method(s)).

Further waiving possibilities

- the viscosity does not have to be determined experimentally if conclusive and consistent literature data are available;
- data for viscosity generated with the same tests and classification principles as specified in the CLP Regulation generated in conjunction with transport classification can satisfy the REACH requirements on a case-by-case basis.

R.7.1.18.5 Impurities; uncertainties

The influence of impurities is negligible if their concentration is below 1 %. The influence of higher concentrations may be significant. There exists no generalised tendency of the influence on the viscosity.

R.7.1.18.6 Endpoint specific information in the registration dossier / in IUCLID**Results and discussion**

- viscosity value and unit according to the used test method;
- preferred units are m Pa s (for dynamic viscosity) and mm²/s (for static viscosity) but other units are also accepted;
- each measured value should be accompanied with temperature (in °C). Usually two values are needed. Preferably one value is measured at approximately 20 °C and another at an approximately 20 °C higher temperature. Two determinations of viscosity should be measured for each temperature;
- for non-Newtonian liquids, the results obtained are preferably in the form of flow curves, which should be interpreted;
- individual and mean values should be provided at each temperature (from OECD Guideline 114 ‘Viscosity of liquids’).

If there are any deviations from the guideline method used or other special considerations then these should be reported. In cases where there is more than one source of data, the endpoint summary under results and discussion should provide a justification for the selection of the key study chapter.

Reference to other ECHA Guidance Documents

Further detailed guidance on viscosity can be found in the following chapters:

IUCLID Section	REACH Annex	Endpoint title	IUCLID 5 End User Manual Chapter	ECHA Practical Guide N.3
4.22	VII 7.17	Viscosity	E.4.23	3.16

R.7.1.19 PARAMETERS ONLY APPEARING IN THE CLP REGULATION

A last group of parameters only appear in the CLP Regulation and have not been introduced into REACH through Article 58 of CLP Regulation. These ones have not to be tested according to the REACH Annex VII criteria, but only and where applicable according to the CLP Regulation. The assignment of hazard classes to relevant subchapters in R.7.1.19 as shown in the table below must therefore only be understood as a means to structure this document in accordance with Annex VII to IX (inclusive) to the REACH Regulation.

1 Table x Information requirements as specified in Annexes VII to IX to REACH, CLP
2 hazards classes and corresponding tests methods according to the Test Method Regulation and CLP

3

REACH Regulation (EC) No. 1907/2006 (the no. in brackets is the respective no. in the table in Annex VII to IX to REACH)	Corresponding test method according to the Test Method Regulation 440/2008	Chapter in revised R.7(a) guidance	CLP Regulation (EC) No. 1272/2008 (the no. in brackets is the respective chapter no. in Annex I to CLP)	Corresponding test method according to the CLP Regulation	Chapter in the <i>Guidance on the Application of the CLP Criteria</i> (ex RIP 3.6)
Not listed in Annex VII to IX to REACH		7.1.19.1 (Parameters only appearing in the CLP Regulation)	Gases under pressure (2.5)		2.6
		7.1.19.2 (Parameters only appearing in the CLP Regulation)	Corrosive to metals (2.16)	UN Test C.1 (section 37.4)	2.15

4

5 **R.7.1.19.1 Gases under pressure**

6 For further guidance please check the *Guidance on the Application of the CLP Criteria* chapter 2.6.

7 **R.7.1.19.2 Corrosive to metals**

8 For further guidance please check the *Guidance on the Application of the CLP Criteria* chapter
9 2.15.

10

1 **R.7.2 Skin- and eye irritation/corrosion and respiratory irritation**

2 **R.7.2.1 Introduction**

3