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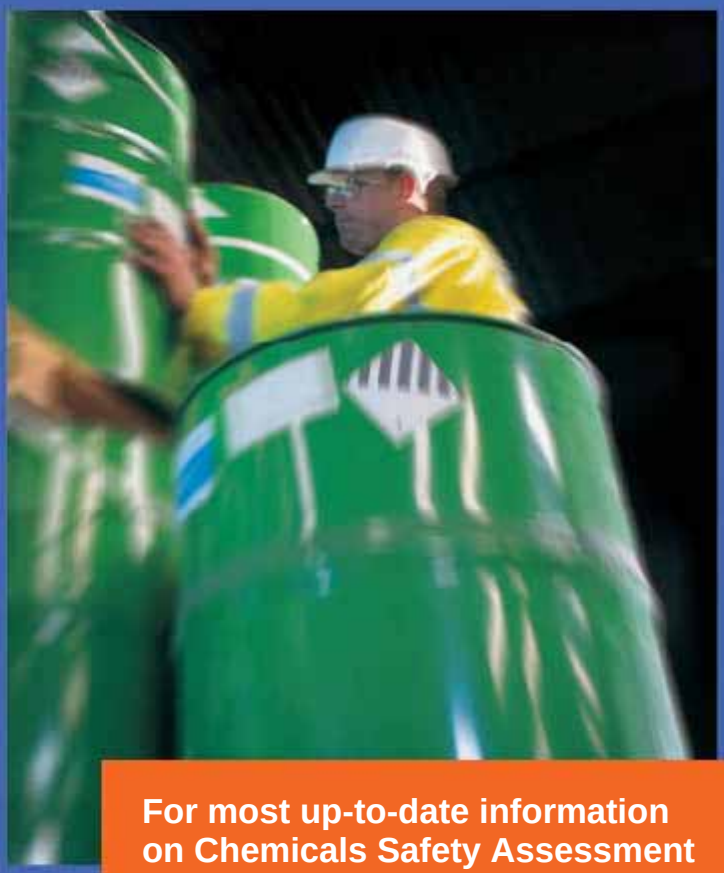
Guidance in a Nutshell

Identification and naming of substances under REACH and CLP



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This document contains guidance on REACH and CLP and provides useful key elements to facilitate compliance with specific requirements under the REACH and CLP Regulations. However, users are reminded that the texts of the REACH and CLP Regulations are 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.

Reference: ECHA-11-B-10-EN
Date: 11/2011
Language: EN

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1. INTRODUCTION

This Guidance in a Nutshell gives a simple and concise introduction on how to identify and name a substance under Regulations (EC) No 1907/2006 (REACH Regulation) and (EC) No 1272/2008 (CLP Regulation).

This Guidance in a Nutshell is aimed at managers and decision-makers of companies producing or importing chemical substances in the European Economic Area[1] (EEA), particularly those belonging to the Small and Medium Enterprises (SME) category. Reading this document will allow them to define the main elements necessary to identify and name substances for REACH and CLP purposes. For details and specific cases they should refer to the full Guidance for identification and naming of substances under REACH and CLP.

This document also gives concise indications of how to assess if substances may be regarded as the same for the purposes of REACH and CLP.

[1] The European Economic Area is composed of Iceland, Liechtenstein, Norway and the 27 European Union Member States.

2. ESSENTIAL TO UNDERSTAND

2.1. Why it is important to clearly identify a substance

The REACH Regulation focuses on substances. Although the provisions of the Regulation apply to the manufacturing, placing on the market or use of substances on their own, in preparations or in articles, the registration requirements apply only to substances.

Unambiguous and clear substance identification is an essential preliminary step in order to comply with the requirements for substances falling under the scope of REACH and to establish whether they fulfil the requirements for exemptions from certain provisions of REACH.

To identify a substance each company needs to use specific identification parameters defined in Annex VI of the REACH Regulation which will be required for different REACH processes. These will be necessary for both companies and authorities in order to carry out their duties and fulfil the requirements of REACH.

Manufactures and importers will need to have properly identified their substances during Substance Information Exchange Fora (SIEFs) formation and for data sharing purposes. The Authorities will need to rely on correct substance identification when they have to carry out a substance evaluation and manage restrictions and authorisation.

Industry also needs to identify substances for CLP, and the same approach as is outlined in this guidance document applies. For notification to the Classification and Labelling inventory applicants have to submit some of the same identification information as required by REACH.

2.2 Definition of “substance” in REACH and CLP

A substance is defined in REACH by *Article 3* and in CLP by *Article 2* as:

“a chemical element and its compounds in the natural state or obtained by any manufacturing process, including any additive necessary to preserve its stability and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition”.

The definition thus goes beyond a pure chemical compound composed of a single molecule. The term covers both substances **obtained by a manufacturing process** and substances in their **natural state** and which can both include several constituents within the substance and to be taken into account as far as possible when identifying the substance for REACH and CLP purposes.

According to REACH and CLP a substance may contain:

- one or more **main constituents**: constituent(s) that make(s) up a significant part of that substance; the main constituent(s) should clearly be other than the following:

- **impurities**: all the unintentional constituents coming from the manufacturing process or from the starting material(s). These could be the result of secondary or incomplete reactions occurring during the production and are present in the final substance even if not sought by the manufacturer.

- **additives**: all the constituents which are intentionally added to stabilise the substance and only for this purpose.

The reader has to carefully consider the difference between a substance and a **mixture.** A mixture consists of several substances. Each individual component substance in a mixture needs to be identified, registered according to REACH and, when required, notified according to CLP either by the substance manufacturer or by the importer of the mixture.

3. WHAT ARE THE TYPES OF SUBSTANCES UNDER REACH AND CLP?

When identifying substances under REACH and CLP the basic rule to be followed is that a substance should be defined as far as possible by the chemical composition (the content of each constituent, the main impurities and any additives) and the chemical identity (name, numerical identifiers, molecular information).

Substances can be divided into two main groups:

3.1 Well-defined substances

When the composition of the substance can be quantitatively and qualitatively defined and the registrant is able to identify all the parameters listed in REACH annex VI, section 2, the substance will be considered as a ***"well defined substance"***. The registrant will be able to identify all the constituents, covering the composition up to 100%. To decide whether it should be considered as **mono-constituent** or instead as **multi-constituent** the so-called ***"80%- 20%"*** and ***"80%-10%" rules*** are applied***.***

If **one constituent** is present at a concentration of **at least 80% (w/w)** and **the impurities** make up **no more than 20% (w/w)**, the substance will be considered as mono-constituent. As noted above intentionally-added substances other than those added to stabilise the substance are separate substances that are not to be considered in the main mass balance.

If **more than one main constituent** is present in a concentration **between 10% and 80% (w/w)** the substance is considered as a multi-constituent substance.

Since it will not always be possible to strictly apply this rule, deviations may be accepted when appropriate. Reasoning based on physico-chemical characteristics or the hazard profile might justify a substance being considered as mono-constituent, even if the main constituent is below 80% or its range of concentration overlaps the 80% criterion.

Furthermore some substances whose composition is fully known may need additional identifiers in order to be unequivocally identified, e.g. crystalline structure, IR absorption peaks or physical or chemical properties. These substances will be named following the same convention as for mono- or multi-constituent substances, but the necessary identification parameters should be added.

3.2 UVCB

There are substances for which the number of constituents is high, or the composition is to a significant extent unknown, or the variability of composition is large or unpredictable. In these cases a straightforward identification is not possible because the substance cannot be sufficiently identified by the chemical composition and it will be considered as a substance of Unknown or Variable composition, Complex reaction products or Biological materials.

Various types of substances can be grouped under the UVCB umbrella. They must be identified by considering the **origin material** of the substance and the most relevant steps during the **manufacturing process**.

Four main sub-types of UVCB have been defined:

UVCB sub-type 1 where the source is biological and the process is synthesis. The biological material is modified by means of a (bio)chemical process resulting in new constituents;

UVCB sub-type 2 where the source is chemical or mineral and new molecules are synthesized by means of (bio)chemical reactions;

UVCB sub-type 3 where the source is biological and the process is a refinement, and new molecules are intentionally generated;

UVCB sub-type 4 where the source is chemical or mineral and the process is a refinement, without intentional chemical reactions.

It is recognised that there will be borderline cases between well-defined and UVCB substances; e.g. substances which are produced by means of reactions between many constituents, each within a broad range, or reaction products with variable and poorly predictable composition. When encountering such unclear cases, the reader is advised to refer to the full Guidance for identification and naming of substances under REACH and CLP.

4 HOW TO IDENTIFY AND NAME A SUBSTANCE

4.1 Requirements for substance identification in REACH

The full identification of a substance under REACH requires the following information:

- **chemical composition** of the substance, considering, where appropriate, impurities and additives besides main constituent(s) and respective typical concentrations and concentration ranges;

- **chemical identity** of the constituent(s) by means of IUPAC name plus other identifiers when available, e.g. EC number, CAS number. For UVCB substances information on the source and manufacturing process is also necessary;

- **molecular and structural information**; this must be defined, when available and appropriate, by molecular and structural formula, information on optical activity, ratio of isomers, molecular weight or molecular weight range;

- **Spectral and analytical data** sufficient to confirm the structure and the composition of the substance.

The data to enable a substance to be identified are listed in section 2 of REACH *Annex VI*. As a general rule, all this information is required regardless of the substance type. However, if it is not technically possible or not scientifically necessary to give a particular piece of information, a reasoned justification should be stated to enable the scientific validity to be assessed.

4.2 Substance naming

The rules to be followed for a correct naming under REACH are related to the substance type as explained in sub-chapters 3.1 and 3.2. For well-defined substances and UVCB substances different approaches and parameters should be considered.

Well-defined mono-constituent substances are named after the main constituent, using its IUPAC name. Other internationally recognized designations may be given as additional information.

Well-defined multi-constituent substances are named as a reaction mass of the main constituents of the substance. The generic format to be used is “Reaction mass of [names of main constituents]”, with the list of constituents presented in alphabetical order and separated by the conjunction “and”.

UVCB substances are named by combining, in this order, source and process. Depending on whether the source is biological or non-biological, the name of the species (genus, species, family) or the starting material (IUPAC name) are to be used. The process must be identified by the chemical reaction, in the case of synthesis of new molecules, or the type of refinement step. In some cases, e.g. for combined processing, more than one single step will need to be specified in addition to the information on the source. There are also borderline cases where UVCB substances could be named based on the constituents.

5. CRITERIA FOR ESTABLISHING IF SUBSTANCES ARE THE SAME

When different manufacturers/importers need to check whether or not their substances can be regarded as the same, they should take into account certain principles. The rules which were applied for establishing EINECS should be regarded as starting points for identifying and naming a substance. For well-defined substances, the rules described in section 3.1 of this document, for mono-constituent substances and for multi-constituent substances are applied.

The consequence of defining a substance as UVCB is that any significant change of source or process would be likely to lead to a different substance (see also section 3.2).

Detailed examples can be found in the relevant chapter of Guidance for identification and naming of substances under REACH and CLP.

6. INQUIRY

For non phase-in substances, or phase-in substances that have not been pre-registered, the potential registrants have the duty to inquire from the Agency whether a registration has already been submitted for the same substance as they intend to register. This inquiry must include information on the identity of the potential registrant, the identity of the substance and on which new studies would be required by the potential registrant to comply with the information requirements.

The Agency will then establish whether the same substance has previously been registered and the result will be communicated to the potential registrant. Any previous or other potential registrants will be informed accordingly.

7. REFERENCES AND FURTHER INFORMATION

This Guidance in a Nutshell provides a summary of key elements necessary to correctly identify a substance. However, it is recommended that before a registration under REACH or notification under CLP is made, particularly in complex cases, manufacturers and importers should consult the full Guidance for identification and naming of substances under REACH and CLP in order to ensure that they correctly define the main elements necessary to identify and name the substance concerned.

The full guidance document provides more detailed examples and explanations of the concepts introduced by the present document. Additional insight may also be gained particularly by consulting the following web pages:

http://esis.jrc.ec.europa.eu/: ESIS the official JRC website where it is possible to search information and EC numbers of substances on EINECS, ELINCS, NLP-list and Annex I 67/548/EEC;

http://iuclid.echa.europa.eu: IUCLID 5 website;

http://www.iupac.org Official site of IUPAC;

http://www.chem.qmul.ac.uk/iupac: Where you can find additional information on chemical nomenclature and recommendations;

http://www.cas.org: The official website CAS registry service can be consulted to retrieve CAS numbers;

http://cactus.nci.nih.gov/services/translate: Free SMILES (Simplified Molecular Input Line Entry Specification) generator.

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