

Substance Identification

HICCS 2008

Helsinki – 20 May 2008

Bernhard Krebs
European Chemicals Agency

Substance Identification



- R = Registration
- E = Evaluation
- A = Authorisation and Restriction of
- CH = Chemicals (\equiv Substances)

Definition according to Article 3(1) of REACH

Substance: means 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

Substance Identification

Manufacturing:

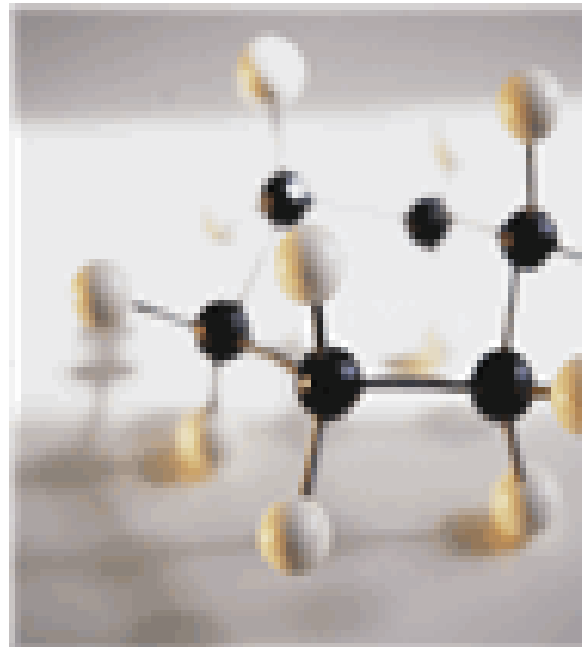
means production or
extraction of a
substance in the
natural state



Substance Identification

Compound \equiv Constituent:

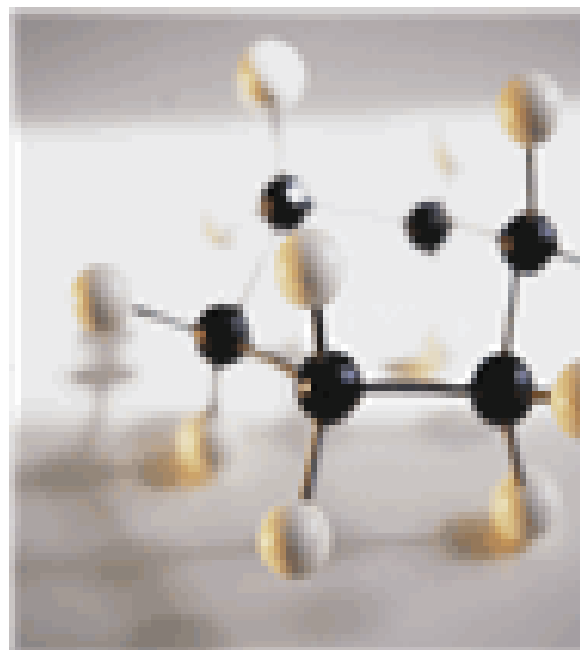
- impurity
- additive
- main constituent



Substance Identification

Impurity:

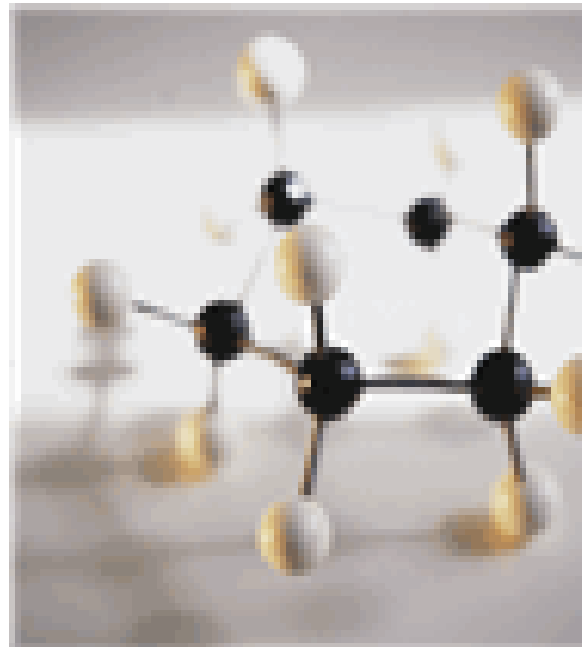
An unintended constituent present in a substance as produced. It may originate from the starting materials or be the result of secondary or incomplete reactions during the production process. While it is present in the final substance it was not intentionally added.



Substance Identification

Additive:

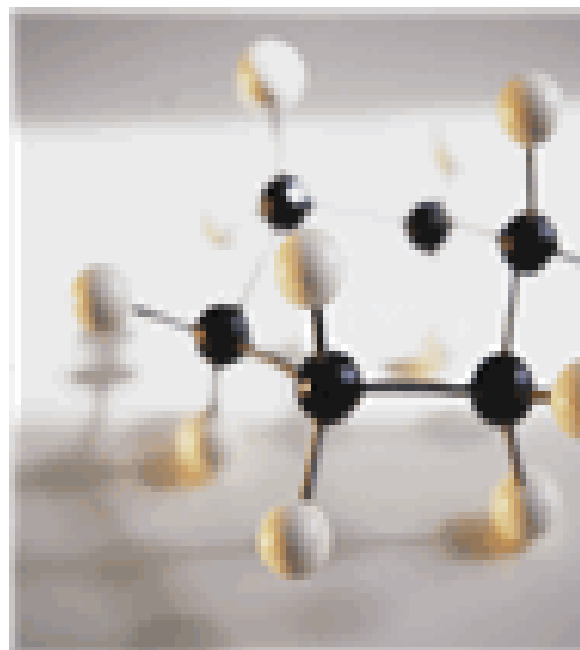
**A substance that has been
intentionally added to stabilise
the substance**



Substance Identification

Main constituent:

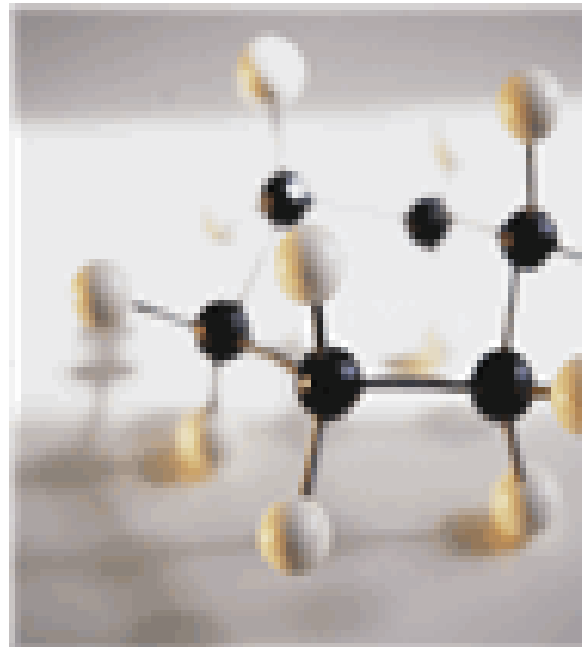
A constituent, not being an additive or impurity, in a substance that makes a significant part of that substance and is therefore used in substance-naming and detailed substance-identification.



Substance Identification

Solvent:

**a liquid constituent capable of dissolving other constituents;
the solvent does not react with the other constituents in forming a solution**



Two 'groups' of substances

- **Substances with defined compositions**
- **UVCB substances**
(Substances of Unknown or Variable composition, Complex reaction products or Biological materials)

Substances with defined compositions

- **Substances with ONE main constituent**

ONE constituent with $\geq 80\%$

→ Substance bears the IUPAC name of this constituent

- **Substances with more main constituents**

Constituents in the range of $\geq 10\%$ and $< 80\%$ are main constituents

→ Substance bears the IUPAC name of these constituents as
'reaction mass of.....'

UVCB-Substances

- **The qualitative and quantitative composition is unknown or variable to a greater or lesser extent**
- **UVCB-substances cannot be defined by their composition (only)**
- **Additional parameters are necessary for describing the substance**

Types of UVCB-Substances

- Defined by the **qualitative** composition only, e.g. linear fatty acids C₈-C₁₆
- Defined by the **organism of origin**, e.g. Aloe vera, Liliaceae, extract
- Defined by the **manufacture / reaction process**, e.g. Alcohols, C₁₆₋₁₈-unsatd., epoxidized
- Defined by the **starting materials**, e.g. 1,3-Isobenzofurandione, reaction products with diethylenetriamine
- **Special UVCB-types**
 - **Petroleum products and Hydrocarbons**, e.g. Hydrocarbons, C₂₆₋₅₅, arom.-rich
 - **Enzymes**, e.g. Dehydrogenase, glucose

Substance Identification



Difference between substance and preparation:

Definition of 'preparation' according to Article 3(2) of REACH:

Preparation means a mixture or solution composed of two or more substances;

Definition of 'substance' according to Article 3(1) of REACH:

Substance: means 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;

Substance Identification



Difference between substance and preparation:

1. **A + C** → **D (95%)** (substance 1)

Substance Identification



Difference between substance and preparation:

1. **A + C → D (95%) (substance 1)**

2. **B + E → F (75%) + R(25%) (substance 2)**

Next step D and (F + R) are mixed together forming D, F and R → preparation

Substance Identification



Difference between substance and preparation:

1. **A + C → D (95%) (substance 1)**

2. **B + E → F (75%) + R (25%) (substance 2)**

In the case:

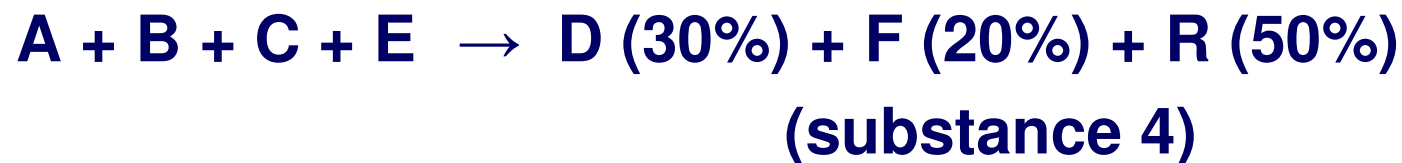
D and (F + R) are mixed together forming

(M (50%) + R (50%)) → substance (substance 3)

Substance Identification



Difference between substance and preparation:



Reaction mass of D; F and R

Substance Identification



What to do for (pre-) registration?

Substance Identification



- Step 1: quantitative analysis of the substance, e.g. chromatography
- Step 2: qualitative analysis of the constituents in the substance – what is in your substance?
- Step 3: apply the guidance for identification and naming of substances under REACH
- Step 4: derive the name of the substance – is the used CAS number correct?
- Step 5: search in EC inventory whether substances is phase-in or not
- Step 6: if phase-in pre-register from 01 June until 01 December 2008
- Step 7: if non-phase-in inquire whether substance was previously registered

Phase-in or non-phase-in substance?

- **Phase-in substances** according to Article 3(20)
 - Listed in European Inventory of Commercial Chemical Substances (EINECS)
 - Manufactured but not places on the market at least once in the 15 years before entry into force
 - No Longer Polymers (NLP)
- **Non-phase-in substances**
 - All other substances which do not meet the criteria above

Substance Identification

Which information is necessary for inquiry?

- Described in Article 26 of the REACH regulation

In particular for the identity of the substance:

- IUPAC name of the substance
- EC number (if available)
- CAS number and name
- Molecular and structural formula
- Degree of purity
- Nature and concentration of impurities and additives
- Spectral data (including recording conditions)
 - UV/VIS (200 – 800 nm)
 - IR (400 – 4000 cm^{-1})
 - NMR (0 – 15 ppm or 0 – 150 ppm)
- Chromatography (including quantitative and qualitative evaluation)
- Any other analytical method used to analyse the substance

Why is substance identification important?

- **Pre-registration**

SIEF-formation → companies find each other

Data sharing

- Animal welfare
- Cost reducing

- **Inquiry**

Companies find each other

Data sharing

- Animal welfare
- Cost reducing