Substance identity - Multiconstituent substances

Lead registrant workshop
2nd February 2012

Sanna Airaksinen
Unit C2 – Substance Identification and Data Sharing

General outline of the substance identification presentations

- Introduction to substance identification
- Substance identity: Multi-constituent substances

- Substance identity: UVCB substances
  (Substances of Unknown or Variable composition, Complex reaction products or Biological materials)
- Conclusions

Aims of this presentation

- To remind about general substance identification issues
- To present specific issues related to multi-constituent substances
  - What is a multi-constituent substance and how they are named
  - What to consider in case of isomeric substances
  - When to register individual constituents of a multi-constituent substance

Introduction to substance identification

- Importance of substance identification:
  Chemical identity is clear
  - What is the substance to be registered
  - Which substances are the same
  - Who has to register jointly
- Substance identity requirements in REACH → Annex VI Section 2
- Types of substances
  - Mono- and multiconstituent substances (well-defined substances)
  - UVCB substances
- Analytical information
  - Analytical information generated on the substance as manufactured
    → specific for each registrant within the joint registration

What is a multi-constituent substance?

- More than one main constituent,
  each main constituent ≥10% but <80% (w/w)
  - Each main constituent completely identified by IUPAC name
  - Typical, min and max concentrations of each constituent reported in composition
  - Concentration ranges specific for each registrant

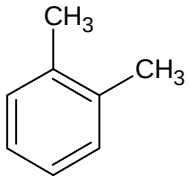
- Generic name format for multi-constituent substance:
  "Reaction mass of [main constituent 1] and [main constituent 2] and …"
  - IUPAC names for main constituents

- Multi-constituent substances in EINECS and in REACH
  - Purposes behind REACH and EINECS different
    → different approach to multi-constituent substances
    EINECS: marketed multi-constituent substance covered by EINECS if all individual constituents were listed
    REACH: if a multi-constituent substance is manufactured/imported it needs to be registered

Borderline case: Mono- or multi-constituent substance?

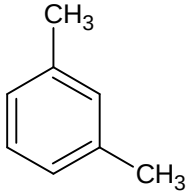
- Typical concentration ≥ 80% but lower concentration limit < 80%
  Typical concentration < 80% but higher concentration limit ≥ 80%
  → possibly mono-constituent
  → possibly multi-constituent

Example



Typical 76%

75 – 95 %



Typical 24%

5 – 25 %

Reaction mass of o-xylene and m-xylene?

Mono-constituent o-xylene with impurity m-xylene?

→ Substance identity is unclear if no justification is given for deviating from the 80% rule

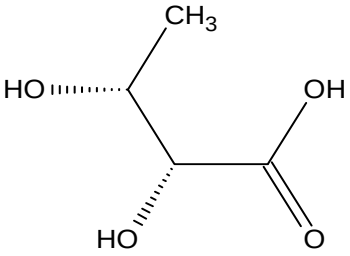
Multi-constituent substances with isomers

- Examples of possible substances
  - Racemate without optical activity
  - Reaction mass of stereoisomers
  - Multiple structural isomers

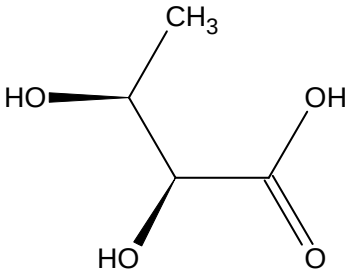
- Unspecific IUPAC name acceptable
  - If all isomers present as main constituents, i.e. ≥10% but <80% (w/w)
- Reaction mass of ...”
  - if not all isomers present ≥ 10%

- Specification of all isomers in composition
- Analytical information should verify the composition; optical activity should be reported (specific rotation value)

Example: Naming of isomeric multi-constituent substances

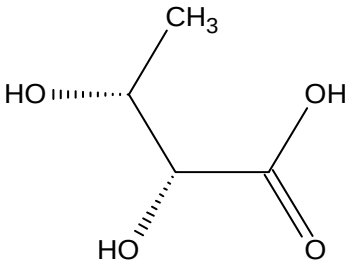


25%

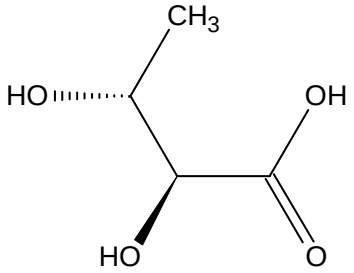


75%

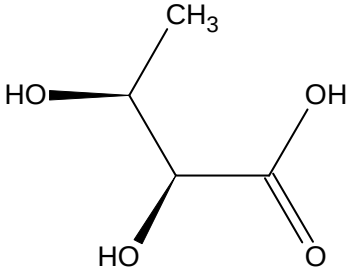
Reaction mass of
(2R,3R)-2,3-dihydroxybutanoic acid and
(2S,3S)-2,3-dihydroxybutanoic acid



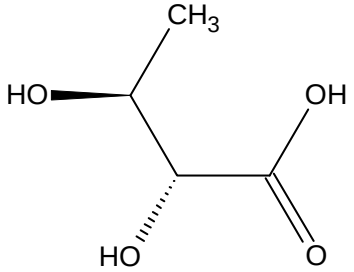
25%



25%



25%



25%

2,3-dihydroxybutanoic acid

Example: Broad EC entry used to identify a substance

- Registered substance identified by generic EC entry
  EC name: 2-Butene, EC number: 203-452-9
  - EC entry for reaction mass of both isomers as main constituents (≥10% but <80%)
    - (E)-but-2-ene, EC number 210-855-3
    - (Z)-but-2-ene, EC number 209-673-7
- Analytical information: only (E)-form present as main constituent
  → generic EC entry too broad

- Generic EC entry does not cover the individual isomers.
  If individual isomers are manufactured, they need to be registered separately.

  → Check that the EC entry does not cover multiple substances

Registration of individual constituents of a multi-constituent substance

- Individual constituents of a multi-constituent substance can be registered separately, if justifiable

- Prerequisites:
  - No reduction in information requirements
  - Sufficient existing data to justify registering individual constituents → no additional testing needed compared to standard approach
  - More efficient situation: lower number of registrations
  - Information on all compositions is given

- Separate analytical information included for all compositions

Thank You!

Sanna Airaksinen
sanna.airaksinen@echa.europa.eu