

Chemicals – substances and mixtures

Identification of chemicals – names and numbers

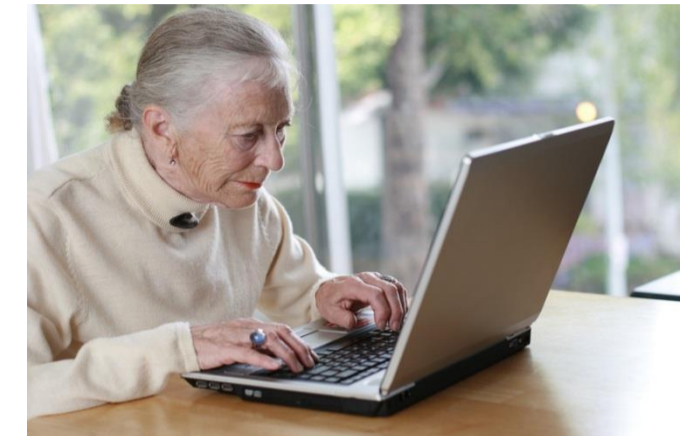
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Crude matter classification

- Products-goods-articles



- Materials



- Chemicals = substances and mixtures



- Substances = well defined or UVCB*



*Unknown or Variable composition, Complex reaction products or Biological materials



A chemical substance - definition

- GHS
- CLP
- Reach
- Wikipedia
- Other?

Substance - Reach and CLP

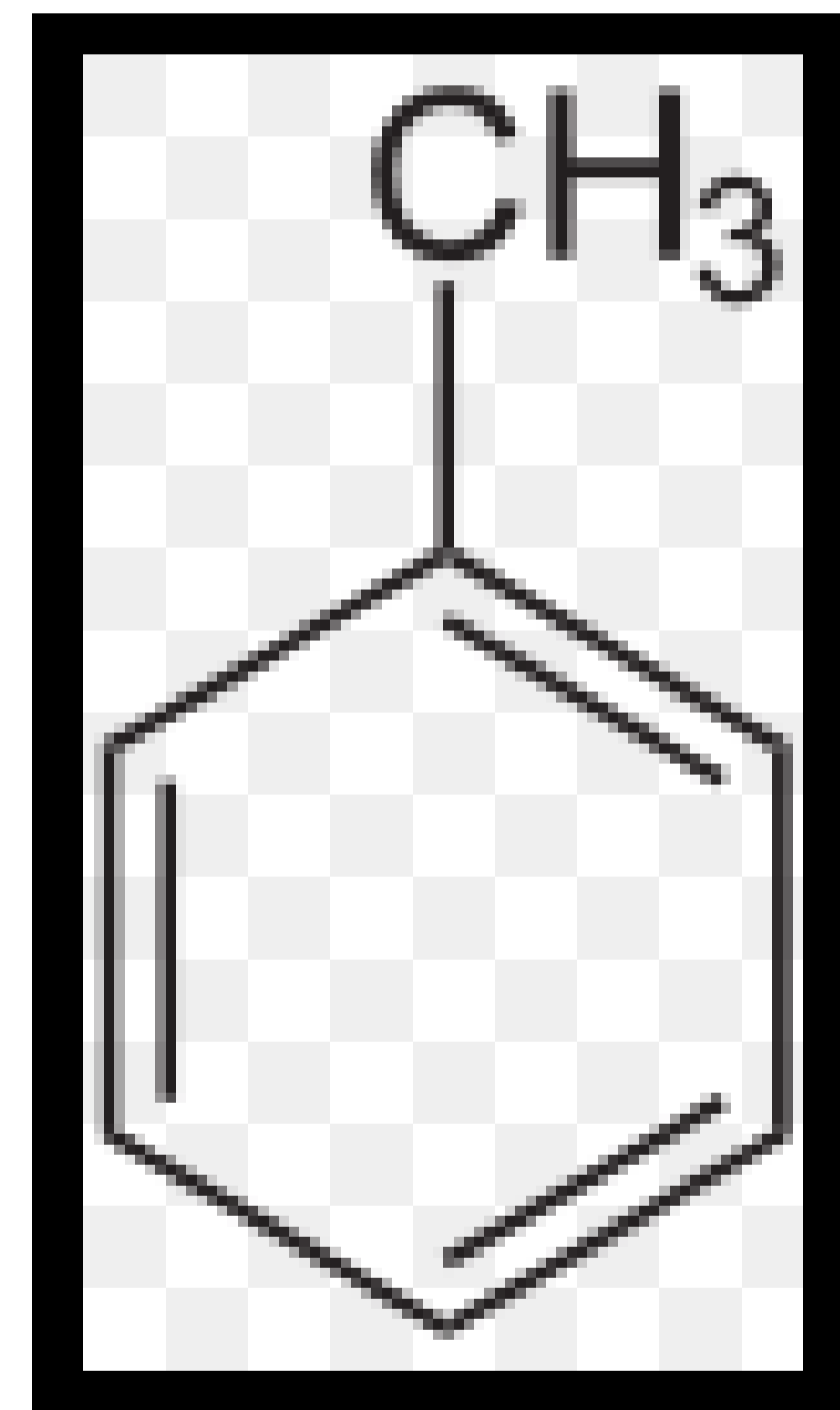
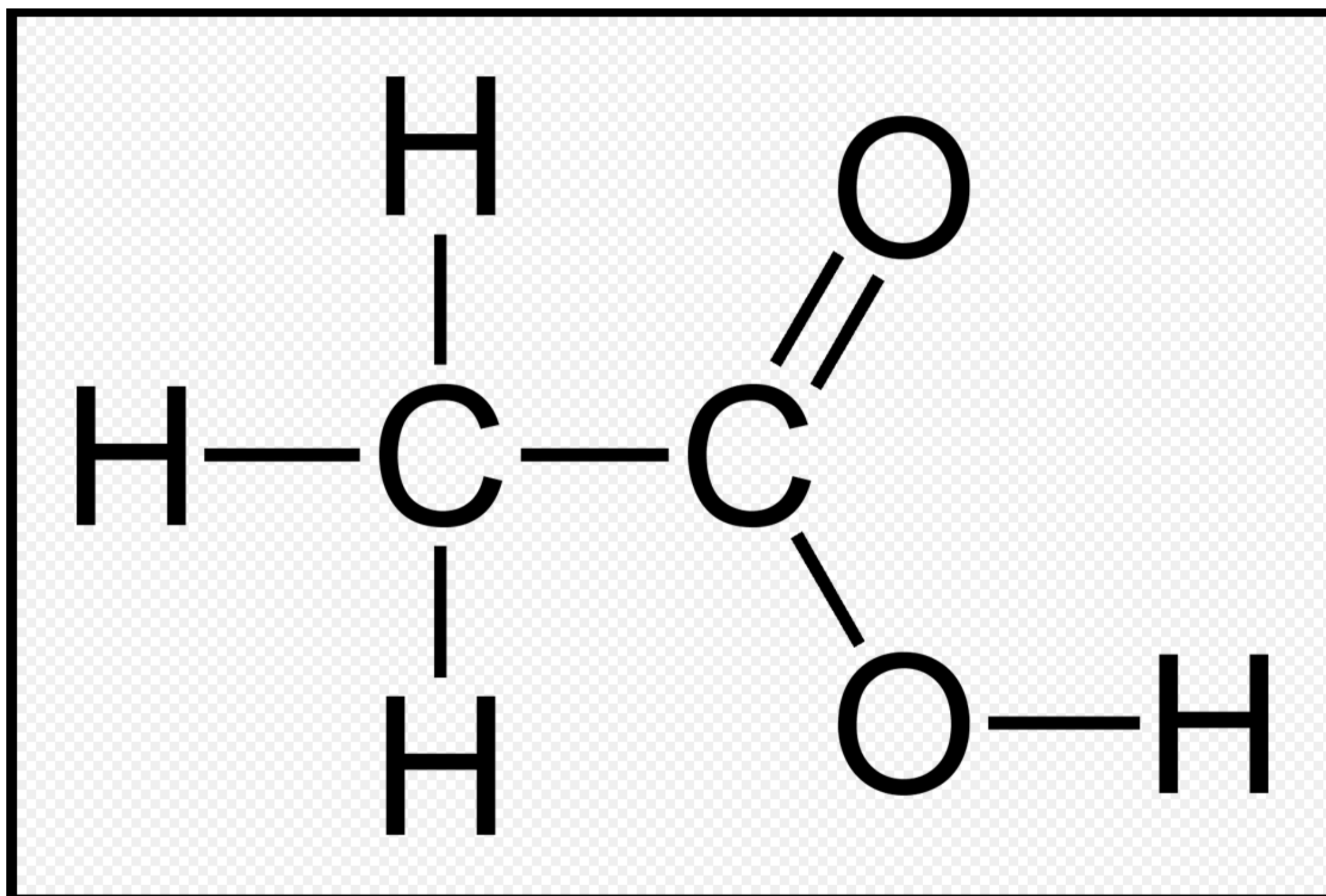
- A substance is defined in Reach by *Article 3* and in CLP by *Article 2* as:
- substance: means a chemical element and its compounds in the natural state or obtained by any manufacturing process, including any additive necessary to preserve its stability and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition;

Mixture

- means a mixture or solution composed of two or more substances

Article

- means an object which during production is given a special shape, surface or design which determines its function to a greater degree than does its chemical composition;



Chemical name

- Acetic acid
- Toluene
 - methylbenzene

IUPAC name [hide]	
Acetic acid ^{[1][2]}	
Systematic name [hide]	
Ethanoic acid ^[3]	
Other names [hide]	
Methanecarboxylic acid ^{[4][5]}	
Identifiers	
Abbreviations	AcOH
CAS number	64-19-7 ✓
PubChem	176
ChemSpider	171 ✓
UNII	Q40Q9N063P ✓
EC number	200-580-7
UN number	2789
DrugBank	DB03166
KEGG	D00010 ✗
MeSH	Acetic+acid
ChEBI	CHEBI:15366 ✓
ChEMBL	CHEMBL539 ✓
IUPHAR ligand	1058
RTECS number	AF1225000
ATC code	G01AD02 ↗ , S02AA10
Beilstein Reference	506007
Gmelin Reference	1380
3DMet	B00009

Many names for the same substance...

- IUPAC
 - trivial name
 - CAS-name
 - ISO name
 - INN name
 - INCI name
 - C.I. name
 - Etc.....
- **Numbers** from different lists and inventories

IUPAC

- International Union for Pure and Applied Chemistry www.iupac.org
- A society of scientists working for standardization in chemistry
- One branch concerns nomenclature

Trivial name

- What is a trivial name?
 - Examples: toluene, phthalic acid
 - The name may be derived from the origin of discovery, like limonene
 - These names often has a history nowadays forgotten



CAS-names are for search in databases

- CAS = Chemical Abstracts Services
a company based in Columbus, Ohio
- Reversed naming by stating the base structure and then adding substituents e.g. Benzene, methyl-
- One Cas-name – one CAS-number – one identity

ISO names for pesticides



- The ISO name is a standardized name used for pesticide substances like Tebuconazole
in systematic IUPAC: [(RS)-1-(4-chlorophenyl)-4,4-dimethyl-3-(1H-1,2,4-triazol-1-ylmethyl)pentan-3-ol]
- 2,4,5-T is also an ISO name [2,4,5-trichlorophenoxyacetic acid]
- More than 1100 of these official pesticide names have been assigned by the International Organization for Standardization (ISO), in accordance with an established system of nomenclature.

INCI names are for cosmetics



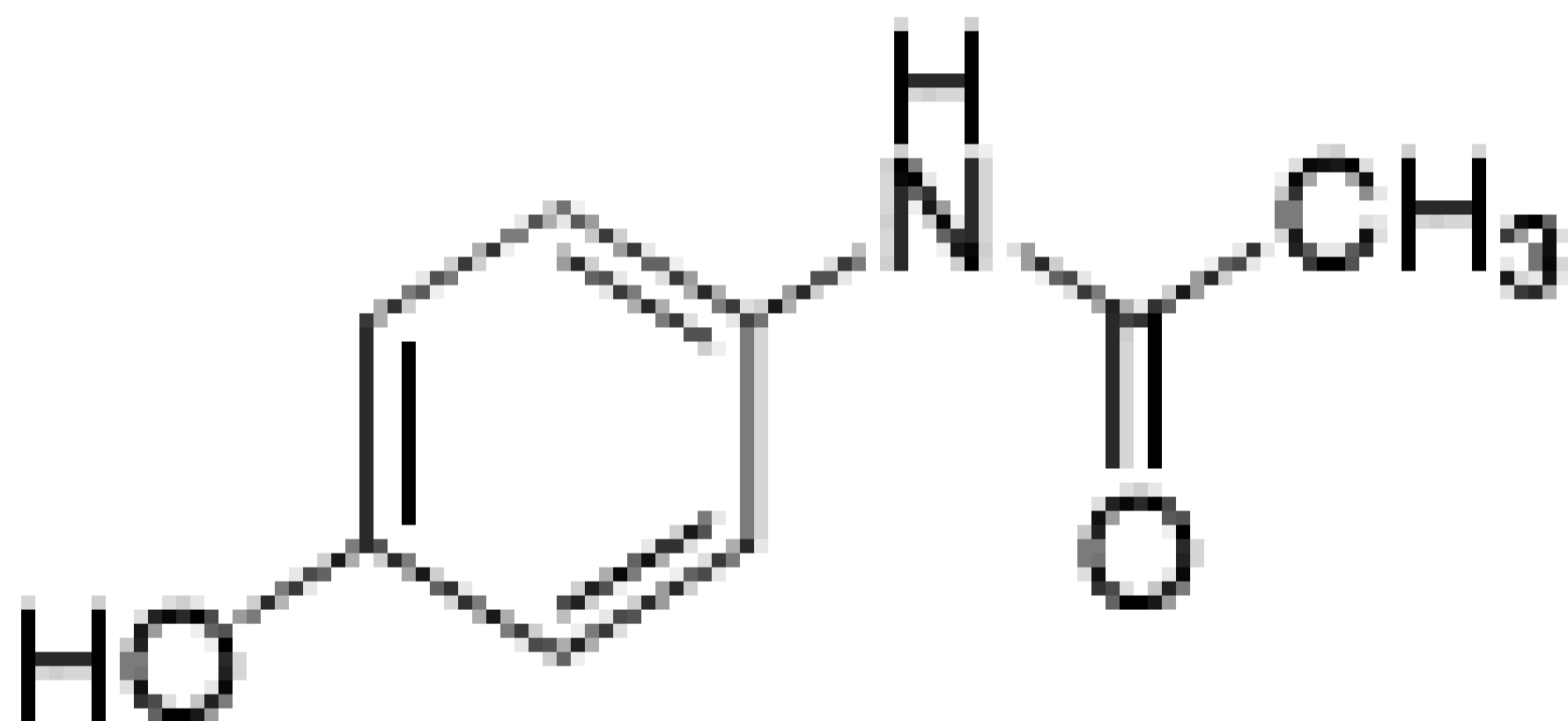
- International Nomenclature of Cosmetic Ingredients
 - The list was started by the EU-authorities in 1993 in cooperation with the branch organisations CTFA in the USA och Colipa in Europe.

- Examples:

<u>INCI Name</u>	<u>CAS Number</u>	<u>Function</u>
Aqua (1714)	7732-18-5	solvent
Polyquaternium-7 (48)	26590-05-6	antistatic

- Since all ingredients of a cosmetic must be given on the label of the product there is a need for a short and accepted nomenclature.
- Polyquaternium-7 (48) = Dimethyldiallylammonium chloride acrylamide polymer

?



INN names are for pharmaceuticals

- An **International Nonproprietary Name (INN)** is the official nonproprietary or generic name given to a pharmaceutical substance, as designated by the World Health Organization (WHO).
- Many naming standards
 - **INN:** paracetamol
 - **British Approved Name (BAN):** paracetamol
 - **United States Adopted Name (USAN):** acetaminophen
 - **Other generic names:** *N*-acetyl-*p*-aminophenol, APAP, *p*-acetamidophenol, acetamol, ...
 - **Proprietary names:** Tylenol, Panadol, Panamax, Perdolan, Calpol, Doliprane, Tachipirina, Ben-u-ron, Atasol, Adol,
 - **IUPAC name:** *N*-(4-hydroxyphenyl)acetamide



C.I. names are for colours



- CI stands for **Colour Index International**, which is a private society of dyers and colourists
- **Commercial name:** 1230 Sunglow Yellow
- **C.I. Constitution numbers:** C.I. 11680
- **C.I. Generic Name:** C.I. Pigment Yellow 1
- IUPAC name: 2-[(4-Methyl-2-nitrophenyl)azo]-3-oxo-N-phenyl butanamide
- Cas-nr: 2512-29-0

Numbers

- CAS-numbers
- CAS , Chemical Abstracts Services
has made abstracts of scientific papers for more than 100 years

An abstract contain key-words

From the 1960s one key-word was a registration number
now recognized as the CAS-number , there are > 85 million numbers

- EC-numbers (EINECS, ELINCS, NPL-list)
- TSCA, MITI , other national inventories
- HS-nomenclature, The Harmonized Commodity
Description and Coding System (HS), "customs tariff no"