Chapter 2 Appendix 2
Detailed Nomenclature Rules

Rolf Bretz

As mentioned, the present SPOLD data exchange software (version 3.0.3) uses only two fields, Name and CAS number, to identify Exchanges. However, the explanatory material to the SPOLD format (in its Annex 44b) contains three fields in the 'Inputs' section: 'Name', 'Specification', and 'CAS number'. The Specification field must be seen as part of the Name field in SPOLD at the moment, because the SPOLD software does not currently support a separate Specification field; it is concatenated to the Name field with one separating blank.

Since a separate 'Specification' field can be foreseen in the coming ISO format, the list of recommended parameters (Appendix A1) already contains the information for this field. The name and the non-formula part of the specification are in one field, separated by commas; the formula and the CAS number are each one in separated fields.

Before a new name is created, it is advisable to search the list in Appendix A1 for similar substances, and name new ones accordingly. New names (as well as the existing ones in Appendix A1) must adhere to the following conventions:

1) General rules:

1a) Capital letters should only be used for the first word in a name unless part of a chemical formula or trade name, where capital letters are a compulsory part of the expression.

1b) The parameter name that gives rise to the least possible misunderstandings is chosen. The name must indicate what is actually measured (especially in sum parameters and indicators).

1c) Very common trivial names that are much shorter or simpler than the systematic names may be used (with great care). Examples: 'Water', 'Acetone', 'Benzo(a)pyrene, 'Methacrylic acid', 'Nitrous oxide'.

1d) Pesticide names that are much shorter or simpler than the systematic names may be used. Examples: 'DDT'.

1e) Ores (mineral resources) are normally expressed as the element that is extracted from them. Example: 'Cadmium Cd, in ground'.

1f) Mixed ores that yield more than one element or other minerals obtain their mineralogic name, rather than a chemical one. Example: 'Chalcopyrite'. Also, ores of different composition or 'richness' can be distinguished by their mineralogic names (and possibly the content of the parent element).

1g) Inorganic anions reported as such (not as salts) carry their trivial names, which also indicate the oxidation level of the central element. Examples: 'Chloride', 'Chlorate'.

1h) Chlorofluorocarbons (CFCs and HCFCs) and Halons must be identified by their CFC/Halon name (cf. 'Special issue: CFCs and HCFCs, p 43), in addition to their chemical name. The CFC/Halon name is appended to the chemical name, separated by comma. Example:'Ethane, 1,1,1, 2-tetrafluoro-, HFC-134a'.

2) Qualifying information in decreasing order of generality, separated by commas:

2a) In names of organics, the 'parent hydride' (Goedkoop and Spriensma 1999), i.e. the principal (unsubstituted) chain or the pre-ferred ring (system) comes first, the substituents follow with their positions, each (including the last one) ending with a hyphen. Example: 'Ethane, 1,1-dichloro-1-fluoro-'.

2b) One characteristic group to be cited as suffix (e.g. sulfonic acid) or functional class name (e.g. nitrile) can follow immediately (without blank) behind the principal chain or ring, before other substituents. Examples: 'Benzenesulfonic acid, hydroxy-', 'Adiponitrile'.

2c) Salts of oxygen-containing acids (inorganic and organic) are considered as derivative of the acid, which appears first. The cation follows, if necessary including its oxidation level, or a counting prefix ('di-', 'tri-'). Examples: 'Sulfuric acid, iron (2+) salt', 'Carbonic acid, disodium salt'.

2d) Esters of organic acids are considered as derivative of the acid, which appears first, followed by the alkyl group, possibly with a counting prefix ('bis-). Example: 'Sebacic acid, bis(2-ethylhexyl) ester'.

2e) Isotopes are named after the parent ele ment[1], followed by a dash and the mass number. Example: 'Cobalt-57'.

2f) Metal ions are named after the parent metal, followed by the word 'ion'. The oxidation level must be indicated, if necessary. Exam ple: 'Chromium, ion (Cr3+)'. Ions are only reported as separate parameters if there are several ones (with different oxidation states), or if they need to be distinguished from the parent metal, e.g. because they have particu lar toxicological or other properties.

2g) Metal oxidation levels that do not form ions per se, but need to be distinguished from others (e.g. because of their toxicity) are named after the parent metal, followed by Roman numerals for the oxidation level. Example: 'Chromium VI'.

2h) Metal oxides and simple salts (sulfides, halogenides, also cyanides[2]) are named after the parent metal, followed by its oxidation level or a counting prefix if necessary and the counter-anion. Examples: 'Chromium trioxide', 'Calcium chloride'.

2i) Metal resources are named after the extracted metal, followed by the words 'in ground'. Example: 'Cadmium, in ground'.

2j) Simple hydrogen compounds follow the same rule as the analogous metal compounds (rule

2h) Examples: 'Hydrogen cyanide', 'Hydrogen peroxide', 'Hydrogen chloride'.

3) Chemical formulae:

3a) Chemical formulae should be given whenever possible, but in a separate field. Any other explanatory information (CFC names, trivial names) follows after the name, separated by a comma. Example: 'Ethane, 2-bromo-2-

---

1 Very common names such as deuterium and tritium can be appended in parentheses, after the atomic symbol. Example: (H-3, Tritium).
2 Cyanides, though having a complex anion CN-, are included here because of historic usage.

chloro-1,1,1-trifluoro-, Halon 2322, Halothane'.

3b) Salt formulae are written conventionally (cations first). Example: 'Na2SO4'.

3c) Formulae of ions indicate the charge (+, ++, 3+; -, --, 3-). In complex anions (which often contain numbers in their formula), a blank is left between formula and charge, to avoid confusion. Example: 'ClO3 -'[3], 'PO4 3-'.

3d) For complicated chemicals, sum formulae can be used.

3e) The sequence of elements (C, H, N, O, P, Br, Cl, F) in sum formulae must be adhered to make the formulae searchable. Examples: 'C3H8NO5P', 'C2HBrClF3'.

3f) Isotope symbols in formulae are derived from the parent element symbol, followed by a dash and the mass number. Example: 'Co-57'.

4) Use of the CAS (Chemical Abstract Service) Registry system (STN 1997):

4a) All Exchanges are first sought in the CAS Registry system (STN 1997). The searching techniques are described in SPOLD (1997). If ever possible, one of the index names registered in CAS has to be used. This needs not be the shortest CAS name; the choice is made according to the rules stated above.

4b) Identifiable, homogeneous chemical substances are always present in the Registry file. The CAS number and the correct chemical formula[4] must be obtained.

4c) Ions and isotopes often have their own CAS numbers (different from the parent element), which have to be used.

4d) Anions can also often be found under their own CAS number, which has to be used.

4e) Materials of unknown or variable composition, complex reaction products, or biological materials sometimes have CAS-Numbers. Example: Alcohols C10-18, ethoxylated, molecular formula unspecified, CAS number 85422-93-1.

4f) Sometimes, chemically identical compounds occur under several different CAS numbers. Example: Malachite (Cu2CO3(OH)2), CAS number 1319-53-5, Copper carbonate hydroxide (Cu2(OH)2CO3) CAS number 12069-69-1. Additional information (e.g. on impurities) has to be collected, to make a proper choice.

As mentioned, the enhanced SPOLD list of parameters (Appendix A1) is not complete in spite of the broad spectrum of databases consulted, and it probably never will be. Therefore, additions to this list must be possible. In order to avoid synonyms and inconsistencies, a set of rules is compiled for amendments to the parameter list:

5) Addition of new exchanges (additions to the parameter list):

5a) Newly added parameters should be meaningful and necessary in actual LCIs. They are not created 'on stock' for theoretical reasons. Example: Not all members of homologous groups or functional classes (e.g. all alcohols, all pesticides, all ores) are added to the list, unless actually used in an inventory (or in an LCIA method, with a separate weighting factor).

5b) New parameters should generally result from direct analytical measurement, and not be calculated from measurements of constituents

---

3 To avoid the false association with "3-", which would indicate a threefold negative charge.
4 Provided that the notation of the formula is compatible with the above rules, otherwise, its notation is adapted (especially the sequence of the elements)

etc. Exception: Sum parameters corrected for overlaps by subtraction (see section 'General rules: corrections to avoid overlap', p 24, and rule 5e below).

5c) Mixtures should only be registered as new parameters if they are determined in one measurement, and if they are homogeneous and reproducible enough to be considered as one parameter. If a main component is known, this should be identified.

5d) Classes of organic chemicals should also only be registered as new parameters if they are determined in one measurement (not summed up from individual species). They are reported under their chemical class name, not as 'Volatile Organic Compounds' with a following classifier, since they may also be emitted to compartments other than air. Example: 'Hydrocarbons, aliphatic, alkanes, linear' (not: 'Volatile Organic Compounds, hydrocarbons, aliphatic, alkanes, linear').

5e) New sum parameters and indicators (naming: see rule 1b) should only be introduced if they result from an existing measurement technique, and not be summed up from individual measurements. Violations of this rule have to be carefully justified. Measured sum parameters must be corrected for overlaps, by subtracting the overlapping individual species that are also reported.

5f) Great care has to be taken to identify new parameters with all available CAS num bers, by thorough searching techniques in the CAS Registry system (STN 1997). If one of the CAS numbers is found in the existing parameter list (Appendix A1), the parameter is not new and may not be added.

5g) As an exception to the precedent rule (5f), ores are named after the extracted element and thus obtain the same CAS number. In rare cases, chemically indistinguishable substances (having the same CAS number) might need to be discriminated in

LCIs. Examples: CO_2 (biogenic vs. fossil), Mg (resource, in ground vs. in sea). Dual CAS numbers in the same category are not allowed in the existing SPOLD software. The solution proposed by SPOLD is to have one entry for CO_2, Mg, etc. and to specify the origin in a different field (Location).

5h) If a new parameter cannot get a CAS number, because it is of unknown or variable composition, a biological material, or a necessary sum parameter or indicator, it has to be named according to rules 1--3. Existing similar or related parameter names in the list have to be carefully examined, to avoid synonymous or overlapping entries. Names analogous to existing parameters should be created if possible, to ensure maximum consistency.

References

Goedkoop M, Spriensma R. 1999. Eco-indicator '99, a damage oriented LCA impact assessment method. Methodology report and Annexe report. publikatiereeks produktenbeleid Nr 1999/36A+B, 2nd revised ed. The Hague and Amersfoort, NL: Ministry of Urban Planning, Housing and the Environment and PRé Consultants. Available at www.pre.nl/ ecoindicator99.

[SPOLD] Society for Promotion of Life-Cycle Assessment Development. 1997. The SPOLD file format '97. Kopenhagen, DK: SPOLD. Available at www.spold.org/publ index.html.

[STN] Scientific and Technical Information Network International. 1997. The CAS Registry file, STN database network. Karlsruhe, DE: Fachinformationszentrum Karlsruhe (FIZ). Available at www.cas.org/stn.html.