IR-1 General Aims, Functions and Methods of Chemical Nomenclature (March 2004)

CONTENTS

IR-1.1 INTRODUCTION

This Chapter provides a brief historical overview of chemical nomenclature followed by a summary of its aims, functions and methods. There are several systems of nomenclature that can be applied to inorganic compounds, briefly described here as an introduction to the later, more detailed, chapters. Because each system can provide a valid name for a compound, a flowchart is presented which should help identify which is the most appropriate for the type of compound of interest. Finally, reference is made to nomenclature recommendations in other areas of chemistry, underlining that inorganic chemistry is part of an integrated whole.

IR-1.2 HISTORY OF CHEMICAL NOMENCLATURE

The activities of alchemy and of the technical arts practised prior to the founding of what we now know as the science of chemistry produced a rich vocabulary for describing chemical substances although the names for individual species gave little indication of composition. However, almost as soon as the true science of chemistry was established a 'system' of chemical nomenclature was developed by Guyton de Morveau in 1782.[1] Guyton's statement of the need for a 'constant method of denomination, which helps the

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intelligence and relieves the memory' clearly defines the basic aims of chemical nomenclature. His system was extended by a joint contribution[2] with Lavoisier, Berthollet, and de Fourcroy and was popularized by Lavoisier.[3] Later, Berzelius championed Lavoisier's ideas, adapting the nomenclature to the Germanic languages,[4] expanding the system and adding many new terms. This system, formulated before the enunciation of the atomic theory by Dalton, was based upon the concept of elements forming compounds with oxygen, the oxides in turn reacting with each other to form salts; the two-word names in some ways resembled the binary system introduced by Linnaeus (Carl von Linné) for plant and animal species.

When atomic theory developed to the point where it was possible to write specific formulae for the various oxides and other binary compounds, names reflecting composition more or less accurately then became common; no names reflecting the composition of the oxosalts were ever adopted, however. As the number of inorganic compounds rapidly grew, the essential pattern of nomenclature was little altered until near the end of the 19th century. As a need arose, a name was proposed and nomenclature grew by accretion rather than by systematization.

When Arrhenius focused attention on ions as well as molecules, it became necessary to name charged particles in addition to neutral species. It was not deemed necessary to develop a new nomenclature for salts; cations were designated by the names of the appropriate metal and anions by a modified name of the non-metal portion.

Along with the theory of coordination, Werner proposed[5] a system of nomenclature for coordination compounds which not only reproduced their compositions but also indicated many of their structures. Werner's system was completely additive in that the names of the ligands were cited, followed by the name of the central atom modified by the suffix 'ate' if the complex was an anion. Werner also used structural descriptors and locants. The additive nomenclature system was capable of expansion and adaptation to new compounds and even to other fields of chemistry.

IR-1.2.1 International cooperation on inorganic nomenclature

In 1892 a conference in Geneva[6] laid the basis for an internationally accepted system of organic nomenclature, but at that time there was nothing comparable for inorganic nomenclature. Thus, many *ad hoc* systems had developed for particular rather than general purposes, and two or more methods often evolved for naming a given compound belonging to a given class. Each name might have value in a specific situation, or be preferred by some users, but there was then the possibility of confusion.

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The need for a uniform practice among English-speaking chemists was recognized as early as 1886 and resulted in agreements on usage by the British and American Chemical Societies. In 1913, the Council of the International Association of Chemical Societies appointed a commission of inorganic and organic nomenclature, but World War I abruptly ended its activities. Work was resumed in 1921 when IUPAC, at its second conference, appointed commissions on the nomenclature of inorganic, organic, and biological chemistry.

The first comprehensive report of the inorganic commission, in 1940,[7] had a major effect on the systematization of inorganic nomenclature and made many chemists aware of the necessity for developing a more fully systematic nomenclature. These IUPAC recommendations were then revised and issued as a small book in 1959[8] followed by a second revision in 1971[9] and a supplement, entitled *How to Name an Inorganic Substance*, in 1977.[10] In 1990 the IUPAC recommendations were again fully revised[11] in order to bring together the many and varied changes which had occurred in the previous 20 years.

Since 1990, more specialized areas have been considered, concerning polyanions,[12] metal complexes of tetrapyrroles (based on Ref. 13), inorganic chain and ring compounds,[14] and graphite intercalation compounds.[15] These topics, together with revised versions of papers on isotopically modified inorganic compounds,[16] hydrides of nitrogen and derived cations, anions and ligands,[17] and regular single-strand and quasi single-strand inorganic and coordination polymers,[18] comprise the seven chapters of *Nomenclature of Inorganic Chemistry II, Recommendations 2000.*[19] A paper entitled *Nomenclature of Organometallic Compounds of the Transition Elements*[20] forms the basis for Chapter IR-10.

IR-1.3 AIMS OF CHEMICAL NOMENCLATURE

The primary aim of chemical nomenclature is simply to provide methodology for assigning descriptors (names and formulae) to chemical substances so that they can be identified without ambiguity, thereby facilitating communication. A subsidiary aim is to achieve standardization. Although this need not be so absolute as to require only one name for a substance, the number of 'acceptable' names needs to be minimized.

When developing a system of nomenclature, public needs and common usage must also be borne in mind. In some cases, the only requirement may be to identify a substance, essentially the requirement prior to the late 18th century. Thus, local names and abbreviations are still used by small groups of specialists. Such local names suffice as long as the specialists understand the devices used for identification. However, this is not nomenclature as defined above since local names do not necessarily convey structural and compositional information to a wider audience. To be widely useful, a nomenclature

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system must be recognisable, unambiguous, and general; the unnecessary use of local names and abbreviations in formal scientific language should therefore be discouraged.

IR-1.4 FUNCTIONS OF CHEMICAL NOMENCLATURE

The first level of nomenclature, beyond the assignment of totally trivial names, gives some systematic information about a substance but does not allow the inference of composition. Most of the common names of the oxoacids (*e.g.* sulfuric acid, perchloric acid) and of their salts are of this type. Such names may be termed semi-systematic and as long as they are for commonly used materials and understood by chemists, they are acceptable. However, it should be recognised that they may hinder compositional understanding by those with limited chemical training.

When a name itself allows the inference of the stoichiometric formula of a compound according to general rules, it becomes truly systematic. Only a name at this second level of nomenclature becomes suitable for retrieval purposes.

The desire to incorporate information concerning the three-dimensional structures of substances has grown rapidly and the systematization of nomenclature has therefore had to expand to a third level of sophistication. Few chemists want to use such a degree of sophistication every time they refer to a compound, but they may wish to do so when appropriate.

A fourth level of nomenclature may be required for the compilation and use of extensive indexes. Because the cost to both compiler and searcher of multiple entries for a given substance may be prohibitive, it becomes necessary to develop systematic hierarchical rules that yield a unique name for a given substance.

IR-1.5 METHODS OF INORGANIC NOMENCLATURE

IR-1.5.1 **Formulation of rules**

The revision of nomenclature is a continuous process as new discoveries make fresh demands on nomenclature systems. IUPAC, through the Division of Chemical Nomenclature and Structure Representation (formed in 2001), studies all aspects of the nomenclature of inorganic and other substances, recommending the most desirable practices to meet specific problems, for example for writing formulae and generating names. New nomenclature rules need to be formulated precisely, to provide a systematic basis for assigning names and formulae within the defined areas of application. As far as possible, however, they should be consistent with existing recommended nomenclature, in both inorganic and other areas of chemistry, and take into account emerging chemistry.

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Recommendations may incorporate common usage when it is systematic and unambiguous; nomenclature developed in isolation from experimental chemistry will be perceived as an imposition and therefore irrelevant to science. At the same time, the development of new rules may also require a more rigorous definition of existing rules to avoid inconsistencies, ambiguities, and the proliferation of names.

IR-1.5.2 Name construction

The systematic naming of an inorganic substance involves the construction of a name from units which are manipulated in accordance with defined procedures to provide compositional and structural information. The element names (or roots derived from them or from their Latin equivalents) (Tables I and II[*], see also Chapter IR-3) are combined with affixes in order to construct systematic names by procedures which are called systems of nomenclature.

There are several accepted systems for the construction of names, as discussed in Section IR-1.5.3. Perhaps the simplest is that used for naming binary substances. This set of rules leads to a name such as iron dichloride for the substance $FeCl_2$; this name involves the juxtaposition of element names (iron, chlorine), their ordering in a specific way (electropositive before electronegative), the modification of an element name to indicate charge (the 'ide' ending designates an elementary anion and, more generally, an element being *treated* formally as anion), and the use of the numerical prefix 'di' to indicate composition.

Whatever the pattern of nomenclature, names are constructed from units which fall into the following classes:

element name roots,
numerical prefixes,
locants,
prefixes indicating atoms or groups – either substituents or ligands,
suffixes indicating charge,
suffixes indicating characteristic substituent groups,
infixes,
additive prefixes,
subtractive suffixes/prefixes,
descriptors (structural, geometric, stereochemical, *etc*.),
punctuation.

The uses of these units are summarized in Chapter IR-2.

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[*] Tables numbered with a Roman numeral are collected together at the end of this book.

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IR-1.5.3 **Systems of nomenclature**

IR-1.5.3.1 *General*

In the development of nomenclature, several systems have emerged for the construction of chemical names; each system has its own inherent logic and set of rules (grammar). Some systems are broadly applicable whereas practice has led to the use of other specialized systems in particular areas of chemistry. The existence of several distinct nomenclature systems leads to logically consistent alternative names for a given substance. Although this flexibility is useful in some contexts, the excessive proliferation of alternatives can hamper communication and even impede trade and legislation procedures. Confusion can also occur when the grammar of one nomenclature system is mistakenly used in another, leading to names that do not represent any given system.

Three systems are of primary importance in inorganic chemistry, namely compositional, substitutive, and additive nomenclature; they are described in more detail in Chapters IR-5, IR-6 and IR-7 respectively. Additive nomenclature is perhaps the most generally applicable in inorganic chemistry, but substitutive nomenclature may be applied in appropriate areas. These two systems require knowledge of the constitution (connectivity) of the compound or species being named. If only the stoichiometry or composition of a compound is known or to be communicated, compositional nomenclature is used.

IR-1.5.3.2 *Compositional nomenclature*

This term is used in the present recommendations to denote name constructions which are based solely on the composition of the substances or species being named, as opposed to systems involving structural information. One such construction is that of a generalised *stoichiometric name*. The names of components which may be themselves elements or composite entities (such as polyatomic ions) are listed with numerical prefixes giving the overall stoichiometry of the compound. If there are two or more components, they are formally divided into two classes, the electropositive and the electronegative components. In this respect, the names are like traditional salt names, although there is no implication about the chemical nature of the species being named.

Grammatical rules are then required to specify the ordering of components, the use of numerical prefixes, and the proper endings for the names of the electronegative components.

Examples:

1. trioxygen, O_3
2. sodium chloride, NaCl
3. phosphorus trichloride. PCl_3

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4. trisodium pentabismuthide, Na_3Bi_5
5. magnesium chloride hydroxide, MgCl(OH)
6. sodium cyanide, NaCN
7. ammonium chloride, NH^4Cl
8. sodium acetate, NaO_2CMe

IR-1.5.3.3 *Substitutive nomenclature*

Substitutive nomenclature is used extensively for organic compounds and is based on the concept of a parent hydride modified by substitution of hydrogen atoms by atoms and/or groups.[21] (In particular it is used for naming organic ligands in the nomenclature of coordination compounds, even though this is an overall additive system.)

It is also used for naming compounds formally derived from the hydrides of certain elements in groups 13-17 of the Periodic Table. Like carbon, these elements form chains and rings which can have many derivatives, and the system avoids the necessity for specifying the hydrogen atoms of the parent hydride.

Rules are required to name parent compounds and substituents, to provide an order of citation of substituent names, and to specify the positions of attachment of substituents.

Examples:

1. 1,1-difluorotrisilane, $SiH_3SiH_2SiHF_2$
2. trichlorophosphane, PCl_3

Replacement operations in which certain non-hydrogen atoms of parents are replaced by different atoms or groups, *e.g.* the skeletal replacements leading to 'a' names in organic chemistry (see Sections P-13.2.1 and P-51.3 of Ref 21), are usually considered as part of substitutive nomenclature and are also used in certain parts of inorganic chemistry.

Example:

3. 1,5-dicarba-*closo*-pentaborane(5), $B_3C_2H_5$
   (CH replacing BH)

Similarly, subtractive nomenclature can be applied in inorganic chemistry, particularly to boron compounds.

Example:

4. 4,5-dicarba-9-debor-*closo*-nonaborate(2–), $[B_6C_2H_8]^{2-}$ (loss of BH)

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IR-1.5.3.4 *Additive nomenclature*

Additive nomenclature treats a compound as a combination of a central atom or central atoms with associated ligands. The particular additive system used for coordination compounds (see Chapter IR-9) is sometimes known as coordination nomenclature although it may be used for much wider classes of compounds, as demonstrated for inorganic acids (Chapter IR-8) and organometallic compounds (Chapter IR-10) and for a large number of simple molecules and ions named in Table IX. Another additive system is well suited for naming chains and rings (Section IR-7.4).

Rules within these systems provide ligand names and guidelines for the order of citation of ligand names and central atom names, designation of charge or unpaired electrons on species, designation of stereochemistry, designation of point of ligation in complicated ligands, *etc.*

Examples:

1. PCl_3, trichloridophosphorus
2. $[CoCl_3(NH_3)_3]$, triamminetrichloridocobalt
3. $H_3SO_4^+$ (= $[SO(OH)_3]^+$), trihydroxidooxidosulfur(1+)
4. $[Pt(\eta^2\text{-}C_2H_4)Cl_3]^-$, trichlorido($\eta^2$-ethene)platinate(1–)
5. $HONH^\bullet$, hydridohydroxidonitrogen(•)
6. $ClSiH_2SiH(Me)NSO$,
   2,2,3-trihydrido-3-methyl-4-azy-1-chlory-6-oxy-2,3-disily-5-sulfy-[6]catena

IR-1.5.3.5 *General naming procedures*

The three basic nomenclature systems may provide different but unequivocal names for a given compound, as demonstrated for PCl_3 above.

The choice between the three depends on the class of inorganic compound under consideration and the degree of detail one wishes to communicate. The following examples further illustrate typical aspects that need to be considered before deciding on a name.

Examples:

1. NO_2

   Would you like simply to specify a compound with this *empirical* formula, or a compound with this *molecular* formula? Would you like to stress that it is a radical? Would you like to specify the connectivity ONO?

2. $Al_2(SO_4)_3\cdot 12H_2O$

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Would you like simply to indicate that this is a compound composed of dialuminium trisulfate and water in the proportion 1:12, or would you like to specify explicitly that it contains hexaaquaaluminium(3+) ions?

3. $H_2P_3O_{10}{}^{3-}$

Would you like to specify that this is triphosphoric acid (as defined in Table IR-8.1) from which three hydrons have been removed? Would you like to specify where the two remaining hydrons are located?

The flowchart shown in Figure IR-1.1 proposes general guidelines for naming compounds and other species.

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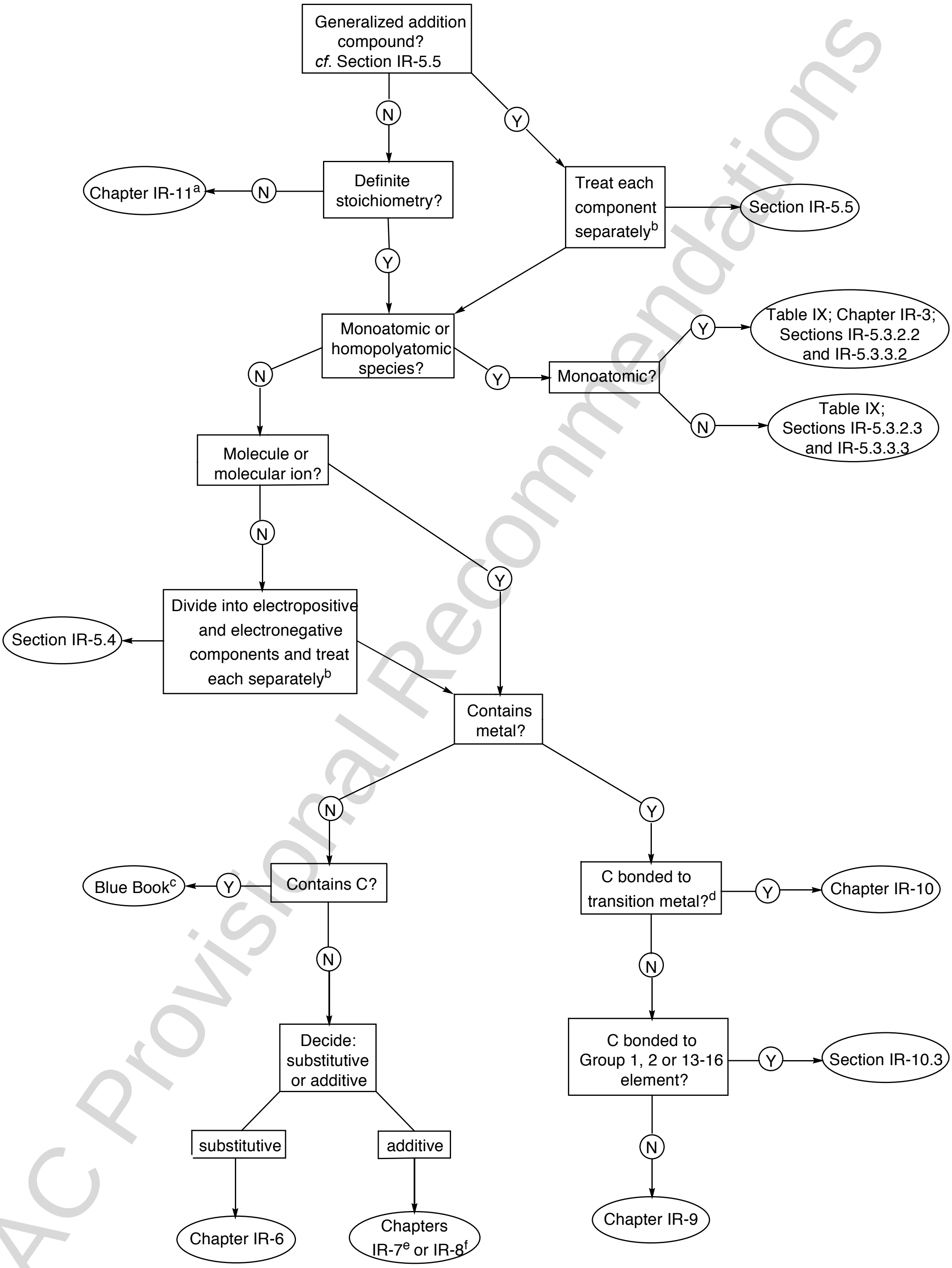
Figure IR-1.1



[a] Chapter IR-11 deals with nomenclature of the solid state. [b] The individual components are named by following the pathway indicated for each of them. The complete name is then assembled according to the recommendations in the Section indicated. [c] In principle, the compound is outside the scope of this book. A few carbon compounds are named in Tables IR-8.1, IR-8.2 and IX, but otherwise the reader is referred to the *Nomenclature of*

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Organic Compounds (the Blue Book*)*. [d] *C*-bonded cyanides are treated as coordination compounds, see Chapter IR-9. [e] The species may be named as a coordination-type compound (Sections IR-7.1 to IR-7.3) or as a chain or ring (Section IR-7.4). [f] For inorganic acids.

IR-1.6 NOMENCLATURE RECOMMENDATIONS IN OTHER AREAS OF CHEMISTRY

Inorganic chemical nomenclature, as inorganic chemistry itself, does not develop in isolation from other fields, and those working in interdisciplinary areas will find useful IUPAC texts on the general principles of chemical nomenclature[22] as well as the specific topics of organic,[21] biochemical,[23] analytical[24] and macromolecular chemistry.[25] Other IUPAC publications include a glossary of terms in bioinorganic chemistry,[26] a compendium of chemical terminology[27] and quantities, units and symbols in physical chemistry.[28] Other texts concerning chemical nomenclature are given in Ref. 29.

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