

IR-8 Inorganic Acids and Derivatives (March 2004)

CONTENTS

- IR-8.1 Introduction and overview
- IR-8.2 General principles for systematic naming of acids
- IR-8.3 Additive names
- IR-8.4 Hydrogen names
- IR-8.5 Abbreviated hydrogen names for certain anions
- IR-8.6 Functional replacement names for derivatives of oxoacids
- IR-8.7 References

IR-8.1 INTRODUCTION AND OVERVIEW

A number of inorganic and simple carbon-containing compounds are commonly given non-systematic or semi-systematic names containing the word 'acid'. Examples are boric acid or orthoboric acid, metaboric acid, fulminic acid, phosphoric acid, diphosphoric acid, *cyclo*-triphosphoric acid, *catena*-triphosphoric acid, dithionous acid, peroxodisulfuric acid or peroxydisulfuric acid, *etc.* These names are unique in modern nomenclature in that, interpreted literally, they describe a particular chemical property of the compounds in question. Systematic names are otherwise based solely on composition and structure.

All such acids may also be given structure-based systematic names using principles already described in preceding chapters on substitutive and additive nomenclature, so in that respect the 'acid'-containing names are superfluous. Furthermore, many species which would be classified as acids based on their chemical properties, are never named as such, *e.g.* aqua ions such as hexaaquaaluminium(3+), and hydrides and derivatives such as ammonium, hydrogen sulfide (sulfane), *etc.* The term 'acid' is thus not used consistently.

Based on these considerations, the use of the word 'acid' in any new name in inorganic nomenclature is discouraged. However, a number of the existing 'acid' names are so commonly used (sulfuric acid, perchloric acid, *etc.*) that it would be unrealistic to suggest replacing them altogether by systematic alternatives. Another reason to include them in the present recommendations is that the acids in question are used as parent structures in the nomenclature of certain organic (*i.e.* carbon-containing) derivatives so that the derivative names are directly or indirectly based on the names containing the word 'acid'. See examples below and Section IR-8.6.

The main purposes of this chapter are:

(a) to show how the inorganic species commonly named as acids may be given systematic additive names (Section IR-8.3 and Tables IR-8.1 and IR-8.2);

(b) to list the 'acid' names that are still allowed due to common usage and/or because they are needed in organic nomenclature (see also, Tables IR-8.1 and IR-8.2).

In addition, Sections IR-8.4 and IR-8.5 deal with a further type of names, denoted here as *hydrogen names*. These names can be viewed as generalisations of common anion names such as 'hydrogencarbonate', but they are not necessary for naming completely specified molecular structures and can be regarded as a special topic.

It is important to understand that although this chapter provides several acceptable names for many inorganic acids, it creates some order in those names; it is left to practitioners to choose the name most suitable for a particular application. In the future, IUPAC aims to provide *preferred* names for inorganic species, including the acids dealt with here, just as Ref. 1 does for organic species.

Finally, names which do not denote compounds of a definite composition, such as 'hydrochloric acid', 'stannic acid', 'tungstic acid', *etc.*, are outside the scope of the systematic nomenclature presented here. However, the chemical systems involved can always be discussed using systematic names such as 'hydrogen chloride', 'tin(IV) oxide', 'tungsten(VI) oxide', *etc.*

A few examples are given now in order to illustrate some of the above general remarks. In these examples, and in the remainder of this chapter, alternative formulae are sometimes provided for clarity in connection with the discussion of additive names. These are based on a perception of the structures in question as generalised coordination entities. For mononuclear entities, this means that the central atom symbol is listed first and then the ligand symbols in alphabetical order, as prescribed in Section IR-4.4.3.2.

Example:

1. phosphoric acid = H_3PO_4 = $[\text{PO}(\text{OH})_3]$.

Based on the structure, the compound can be named additively (Chapter IR-7) as trihydroxidooxidophosphorus or substitutively (Chapter IR-6) as a derivative of the parent hydride λ^5 -phosphane (PH_5), leading to the name trihydroxy- λ^5 -phosphane.

As opposed to the two latter names, the name 'phosphoric acid' does not convey the structure, but does fit into a general pattern whereby the ending 'ic' denotes a higher or the highest

possible oxidation state (compare 'nitric acid', 'sulfuric acid'). Examples 2 and 3 show organic derivatives named on the basis of phosphoric acid as the parent.

Examples:

- | | | |
|----|-----------------------------|-------------------------------|
| 2. | $\text{PO}(\text{OMe})_3$ | trimethyl phosphate |
| 3. | $\text{PO}(\text{NMe}_2)_3$ | hexamethylphosphoric triamide |

Each of these two compounds could also be named substitutively, on the basis of the above parent hydride, or additively, but the names given here are preferred IUPAC names (see Sections P-67.1.2.4 and P-67.1.3.1 of Ref. 1).

Some organic derivative names still contain the word 'acid', as in the following derivatives of arsonic acid = $\text{H}_2\text{AsHO}_3 = [\text{AsHO}(\text{OH})_2]$.

Examples:

- | | | |
|----|------------------------------------|--|
| 4. | $\text{PhAsO}(\text{OH})_2$ | phenylarsonic acid |
| 5. | $\text{EtAsCl}(\text{OH})\text{S}$ | ethylarsonochloridothioic <i>O</i> -acid |

The name in Example 4 regards the compound as derived from arsonic acid, by substitution of a phenyl group for the hydrogen atom bound directly to arsenic. The name in Example 5, in addition to the hydrogen substitution, involves functional replacement nomenclature (Section IR-8.6).

Note that there is one general case where the word 'acid' may appear in a fully systematic name of an inorganic compound, namely when substitutive nomenclature is used and prescribes a suffix for the highest ranking substituent group which ends with the word 'acid'.

Consider the polythionic acids, $\text{H}_2\text{S}_n\text{O}_6 = [(\text{HO})(\text{O})_2\text{SS}_{n-2}\text{S}(\text{O})_2(\text{OH})]$ ($n \geq 2$), which have the common names 'dithionic acid', 'trithionic acid', 'tetrathionic acid', *etc.* They may be named systematically using additive nomenclature, as shown in Table IR-8.1. For $n \geq 3$, they may also be named substitutively on the basis of the central (poly)sulfane skeleton, as exemplified below.

Examples:

- | | | |
|----|--|---------------------------|
| 6. | $\text{H}_2\text{S}_3\text{O}_6 = [(\text{HO})(\text{O})_2\text{SSS}(\text{O})_2(\text{OH})]$ | sulfanedisulfonic acid |
| 7. | $\text{H}_2\text{S}_4\text{O}_6 = [(\text{HO})(\text{O})_2\text{SSSS}(\text{O})_2(\text{OH})]$ | disulfanedisulfonic acid, |

Table IR-8.1 Acceptable common names and fully systematic (additive) names for oxoacid and related structures.

(Insert separate landscape Table)

IR-8.2 GENERAL PRINCIPLES FOR SYSTEMATIC NAMING OF ACIDS

Molecular compounds and ions commonly viewed as inorganic acids are treated no differently from other molecular species when constructing systematic names.

The most easily applied general principle for systematic naming is that of additive nomenclature, exemplified in Section IR-8.3. As mentioned in IR-8.1, substitutive nomenclature could also be generally applied. However, this is not further elaborated here.

Sections IR-8.4 and IR-8.5 describe hydrogen names, which are related to additive names and only needed in special cases.

The method called 'acid nomenclature' in Section I-9.6 of Ref. 2 is little used and not needed. Its use is therefore no longer recommended.

IR-8.3 ADDITIVE NAMES

Molecules or ions that can *formally* be regarded as mononuclear coordination entities may be named additively, applying the rules described in Chapter IR-7.

Examples:

- | | | |
|----|--|------------------------------|
| 1. | $\text{H}_3\text{SO}_4^+ = [\text{SO}(\text{OH})_3]^+$ | trihydroxidooxidosulfur(1+) |
| 2. | $\text{H}_2\text{SO}_4 = [\text{SO}_2(\text{OH})_2]$ | dihydroxidodioxidosulfur |
| 3. | $\text{HSO}_4^- = [\text{SO}_3(\text{OH})]^-$ | hydroxidotrioxidosulfate(1-) |

Structures which can be regarded as oligonuclear coordination entities may be named as such (Section IR-7.3) or may be named using the system for inorganic chains and rings (Section IR-7.4).

In principle, the choice of method in the latter case is arbitrary. However, the machinery of coordination compound nomenclature was developed to enable the handling of complex structures involving polyatomic, and particularly polydentate, ligands and sometimes multiply bridging ligands. Furthermore, the separation into ligands and central atoms, obvious in compounds most usually classified as coordination compounds, may be less obvious in the polyoxoacids. Thus, additive nomenclature of the coordination type tends to be more intricate than necessary when naming polyoxoacids forming relatively simple chains and rings. Here

the chains and rings system is easily applied, and the names so derived are easy to decipher. However, this system can lead to long names with many locants.

Both types of additive names are exemplified below for oligonuclear systems.

Examples:

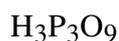
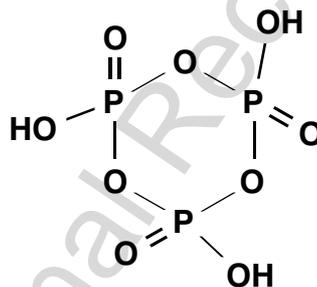
4. The compound commonly named diphosphoric acid, $\text{H}_4\text{P}_2\text{O}_7 = [(\text{HO})_2\text{P}(\text{O})\text{OP}(\text{O})(\text{OH})_2]$, is named according to the coordination-type additive nomenclature as:

μ -oxido-bis[dihydroxidooxidophosphorus]

or as a five-membered chain with ligands:

1,5-dihydrido-2,4-dihydroxido-2,4-dioxido-1,3,5-trioxy-2,4-diphosphy-[5]catena

5. The compound commonly named *cyclo*-triphosphoric acid:



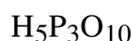
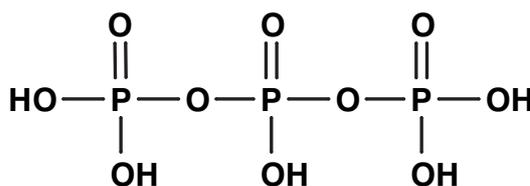
may be named according to coordination-type additive nomenclature as:

tri- μ -oxido-tris(hydroxidooxidophosphorus),

or as a six-membered ring with ligands:

2,4,6-trihydroxido-2,4,6-trioxido-1,3,5-trioxy-2,4,6-triphosphy-[6]cycle

6. The related compound, *catena*-triphosphoric acid,



may be named as a trinuclear coordination entity:

pentahydroxido-1 κ^2 O,2 κ O,3 κ^2 O-di- μ -oxido-trioxido-1 κ O,2 κ O,3 κ O-triphosphorus,

or as a symmetrical dinuclear coordination entity with a bridging phosphate ligand:

μ -[hydroxidotrioxidophosphato(2-)-1 κ O,2 κ O]-bis(dihydroxidooxidophosphorus),

or as a mononuclear coordination entity with two phosphate ligands:

bis(dihydroxidodioxidophosphato)hydroxidooxidophosphorus,

or as a seven-membered chain with ligands:

1,7-dihydrido-2,4,6-trihydroxido-2,4,6-trioxido-1,3,5,7-tetraoxy-2,4,6-triphosphy-[7]catena.

All inorganic oxoacids for which a common name containing the word 'acid' is still acceptable according to the present recommendations (and in many cases used as a parent in functional nomenclature, as described in Section IR-8.1) are listed in Table IR-8.1 together with additive names to illustrate how systematic names may be given.

Several names omitted from Ref. 2, *e.g.* selenic acid and hypobromous acid, are reinstated because they are unambiguous and remain in common use (including their use as parent names in replacement nomenclature).

Table IR-8.1 also includes anions derived from the neutral oxoacids by successive dehydration. Many of these anions also have common names that are still allowed, in some cases in spite of the fact that they are based on nomenclature principles that are now otherwise abandoned (*e.g.* nitrate/nitrite and perchlorate/chlorate/chlorite/hypochlorite). For names involving the prefix 'hydrogen', see Sections IR-8.4 and IR-8.5.

It is important to note that the presence of a structure in Table IR-8.1 does not imply that the structure has been described in the literature or that there has been a need to name it in the past. Several names are included only for completeness and to make parent names available for naming organic derivatives.

IR-8.4 HYDROGEN NAMES

An alternative nomenclature for hydrogen-containing compounds and ions is described here. The word 'hydrogen', with a numerical prefix if relevant, is joined (with no space) to an anion name formed by additive nomenclature and placed within appropriate enclosing marks (see Section IR-2.2). This construction is followed (again with no space) by a charge number

indicating the total charge of the species or structural unit being named (except for neutral species/units).

Hydrogen names are useful when the connectivity (the positions of attachment of the hydrons) in a hydron-containing compound or ion is unknown or not specified (*i.e.* when which of two or more tautomers is not specified, or when one does not wish to specify a complex connectivity, such as in network compounds).

Some of the following examples are discussed in detail below.

Examples:

1. $\text{H}_2\text{P}_2\text{O}_7^{2-}$ dihydrogen(heptaoxidodiphosphate)(2-)
2. $\text{H}_2\text{B}_2(\text{O}_2)_2(\text{OH})_4$ dihydrogen(tetrahydroxidodi- μ -peroxido-diborate)
3. $\text{H}_2\text{Mo}_6\text{O}_{19} = \text{H}_2[\text{Mo}_6\text{O}_{19}]$ dihydrogen(nonadecaoxidohexamolybdate)
4. $\text{H}_4[\text{SiW}_{12}\text{O}_{40}] = \text{H}_4[\text{W}_{12}\text{O}_{36}(\text{SiO}_4)]$
tetrahydrogen[(tetracontaoxidosilicododecatungsten)ate], or
tetrahydrogen[hexatriacontaoxido(tetraoxidosilicato)dodecatungstate], or
tetrahydrogen(silicododecatungstate)
5. $\text{H}_4[\text{PMo}_{12}\text{O}_{40}] = \text{H}_4[\text{Mo}_{12}\text{O}_{36}(\text{PO}_4)]$
tetrahydrogen[tetracontaoxido(phosphorusdodecamolybdenum)ate], or
tetrahydrogen[hexatriacontaoxido(tetraoxidophosphato)dodecamolybdate], or
tetrahydrogen(phosphododecamolybdate)
6. $\text{H}_6[\text{P}_2\text{W}_{18}\text{O}_{62}] = \text{H}_6[\text{W}_{18}\text{O}_{54}(\text{PO}_4)_2]$
hexahydrogen[dohexacontaoxido(diphosphorusoctadecatungsten)ate], or
hexahydrogen[tetrapentacontaoxidobis(tetraoxidophosphato)octadecatungstate], or
hexahydrogen(diphosphooctadecatungstate)
7. $\text{H}_4\text{Fe}(\text{CN})_6$ tetrahydrogen(hexacyanidoferrate)
8. $\text{H}_2\text{PtCl}_6 \cdot 2\text{H}_2\text{O}$ dihydrogen(hexachloridoplatinate)—water (1/2)
9. HCN hydrogen(nitridocarbonate)

In Example 1, the two hydrons could be located either on two oxygen atoms on the same phosphorus atom or one on each of the phosphorus atoms. Thus, as already indicated, hydrogen names do not necessarily fully specify the structure.

In the same way, the hydrogen name in Example 9 covers, in principle, two tautomers. This also applies to the common compositional name 'hydrogen cyanide'. The names 'hydridonitridocarbon' (additive nomenclature), 'methylidyneazane' (substitutive

nomenclature) and 'formonitrile' (functional organic nomenclature) all specify the tautomer HCN.

Hydrogen names may also be used for molecular compounds and ions with no tautomerism problems if one wishes to emphasise the conception of the structure as hydrons attached to the anion in question:

Examples:

10.	HMnO ₄	hydrogen(tetraoxidomanganate)
11.	H ₂ MnO ₄	dihydrogen(tetraoxidomanganate)
12.	H ₂ CrO ₄	dihydrogen(tetraoxidochromate)
13.	HCrO ₄ ⁻	hydrogen(tetraoxidochromate)(1-)
14.	H ₂ Cr ₂ O ₇	dihydrogen(heptaoxidodichromate)
15.	H ₂ O ₂	dihydrogen(peroxide)
16.	HO ₂ ⁻	hydrogen(peroxide)(1-)
17.	H ₂ S	dihydrogen(sulfide)
18.	H ₂ NO ₃ ⁺	dihydrogen(trioxidonitrate)(1+)

Note the difference from *compositional names* such as 'hydrogen peroxide' for H₂O₂ and 'hydrogen sulfide' for H₂S (Chapter IR-5) in which (in English) there is a space between the electropositive and electronegative component(s) of the name.

Compositional names of the above type, containing the word 'hydrogen', were classified as 'hydrogen nomenclature' in the discussion of oxoacids in Section I-9.5 of Ref. 2, and such names were extensively exemplified. However, in order to avoid ambiguity, their general use is not encouraged here. Consider, for example, that the compositional names 'hydrogen sulfide' and 'hydrogen sulfide(2-)' can both be interpreted as H₂S as well as HS⁻. The situation with H₂S is completely analogous to that with Na₂S which may be named sodium sulfide, disodium sulfide, sodium sulfide(2-) and disodium sulfide(2-), except that in the latter case misinterpretation of the first and third names as denoting NaS⁻ is improbable. In Ref. 2, the names 'hydrogensulfide(1-)' and 'monohydrogensulfide' for HS⁻ were proposed to avoid ambiguity. (However, in some languages there is no space in compositional names so that very delicate distinctions are required anyway.)

The strict definition of *hydrogen names* proposed here is meant to eliminate such confusion by imposing the requirements:

- (i) that 'hydrogen' be attached to the rest of the name,
- (ii) that the number of hydrogens must be specified by a multiplicative prefix,
- (iii) that the anionic part be placed in enclosing marks, and

(iv) that the charge of the total structure being named is specified.

Hydrogen names constructed in this way cannot be mistaken for other types of name.

The only allowed exceptions to the above format for hydrogen names are the few particular abbreviated anion names listed in Section IR-8.5.

In a few cases, no confusion can arise, and the distinction between compositional name and hydrogen name is not as important, most notably for the hydrogen halides. Thus, HCl can equally unambiguously be named 'hydrogen chloride' (compositional name) and 'hydrogen(chloride)' (hydrogen name).

Examples 1, 3-6 and 14 above demonstrate that homo- and heteropolyoxoacids and their partially dehydrated forms can be given hydrogen names once the corresponding anions have been named. Examples 4-6 each feature three alternatives. The first two names are both fully additive for the anion part and correspond to different ways of dissecting the structure into ligands and central atoms. The last names, involving the prefixes 'silico' and 'phospho', are examples of a common semi-systematic nomenclature which is not recommended for general use because it requires complex conventions in order to be unambiguous.

Rules for naming very complicated homo- and heteropolyoxoanions are given in Chapter II-1 of Ref. 3.

Note that Examples 10-14 above show how one may easily name transition metal compounds that have been named as acids in the past. Names such as permanganic acid, dichromic acid, *etc.*, are not included in the present recommendations because they represent an area where it is difficult to systematise and decide what to include, and where the names are not needed for organic nomenclature, as opposed to the corresponding 'acid' names for acids of main group elements.

Finally, note that usage is different from the above in the names of salts and partial esters of organic polyvalent acids, where 'hydrogen' is always cited as a separate word just before the anion name, *e.g.* 'potassium hydrogen phthalate' or 'ethyl hydrogen phthalate'.

IR-8.5 ABBREVIATED HYDROGEN NAMES FOR CERTAIN ANIONS

A few common anionic species have names which can be regarded as short forms of hydrogen names formed according to the above method. These names, all in one word without explicit indication of the molecular charge, and without the enclosing marks, are

accepted due to their brevity and long usage and because they are not ambiguous. It is strongly recommended that this list be viewed as limiting due to the ambiguities that may arise in many other cases, *cf.* the discussion in Section IR-8.4.

<i>Anion</i>	<i>Accepted simplified hydrogen name</i>	<i>Hydrogen name</i>
H_2BO_3^-	dihydrogenborate	dihydrogen(trioxidoborate)(1-)
HBO_3^{2-}	hydrogenborate	hydrogen(trioxidoborate)(1-)
HSO_4^-	hydrogensulfate	hydrogen(tetraoxidosulfate)(1-)
HCO_3^-	hydrogencarbonate	hydrogen(trioxidocarbonate)(1-)
H_2PO_4^-	dihydrogenphosphate	dihydrogen(tetraoxidophosphate)(1-)
HPO_4^{2-}	hydrogenphosphate	hydrogen(tetraoxidophosphate)(2-)
H_2PO_3^-	dihydrogenphosphite	dihydrogen(trioxidophosphate)(2-)
HPO_3^{2-}	hydrogenphosphite	hydrogen(trioxidophosphate)(1-)
H_2PO_3^-	dihydrogenphosphite	dihydrogen(trioxidophosphate)(2-)
HPO_3^{2-}	hydrogenphosphite	hydrogen(trioxidophosphate)(1-)
HSO_4^-	hydrogensulfate	hydrogen(tetraoxidosulfate)(1-)
HSO_3^-	hydrogensulfite	hydrogen(trioxidosulfate)(1-)

IR-8.6 FUNCTIONAL REPLACEMENT NAMES FOR DERIVATIVES OF OXOACIDS

In functional replacement nomenclature, substitution of =O or -OH groups in parent oxoacids (such as $\text{O} \rightarrow \text{S}$, $\text{O} \rightarrow \text{OO}$, $\text{OH} \rightarrow \text{Cl}$, *etc.*) is indicated by the use of infixes as exemplified below (*cf.* Ref. 1, Section P-67.1.2.1).

<i>Replacement operation</i>	<i>Infix</i>
$\text{OH} \rightarrow \text{NH}_2$	amid(o)
$\text{O} \rightarrow \text{OO}$	peroxo
$\text{O} \rightarrow \text{S}$	thio
$\text{O} \rightarrow \text{Se}$	seleno
$\text{O} \rightarrow \text{Te}$	telluro
$\text{OH} \rightarrow \text{F}$	fluorid(o)
$\text{OH} \rightarrow \text{Cl}$	chlorid(o)
$\text{OH} \rightarrow \text{Br}$	bromid(o)
$\text{OH} \rightarrow \text{I}$	iodid(o)
$\text{OH} \rightarrow \text{CN}$	cyanid(o)

Example 5 in Section IR-8.1 demonstrates the use of the prefixes for OH → Cl and O → S to arrive at the name 'arsonochloridothioic *O*-acid' for the derived parent $\text{HAsCl(OH)S} = [\text{AsClH(OH)S}]$, required for naming the organic derivative:

EtAsCl(OH)S ethylarsonochloridothioic *O*-acid.

Functional replacement names may, of course, be used for the derived parent acids themselves. However, since this amounts to introducing an additional system which is not needed, such names are not recommended for general use in inorganic nomenclature. As mentioned above, additive and substitutive nomenclature can always be used.

Example:

1. $\text{HAsCl(OH)S} = [\text{AsClH(OH)S}]$
chloridohydrido(hydroxido)(sulfido)arsenic (additive), or
chloro(hydroxy)- λ^5 -arsanethione (substitutive)

Nevertheless, in Table IR-8.2 several inorganic structures are listed which can be regarded as derived from structures in Table IR-8.1 by various replacement operations. Acceptable common names are given which are sometimes based on a variation of the above system using a prefix instead of an infix (*e.g.* 'thiosulfuric acid' rather than 'sulfurothioic acid'). The prefix variant is accepted only in these specific cases.

Table IR-8.2 Common names, functional replacement names, and fully systematic (additive) names for some functional replacement derivatives of oxoacids.

(Insert separate landscape Table)

A problem that would arise with general use of the prefix variant of functional replacement names is illustrated by the thio acids. The names 'trithiocarbonic acid', 'tetrathiophosphoric acid', *etc.*, would lead to anion names 'trithiocarbonate', 'tetrathiophosphate', *etc.*, which appear to be additive names but are incorrect because the ligand prefix is now 'sulfido' or 'sulfanedido' [thus giving 'trisulfidocarbonate(2-)', 'tetrasulfidophosphate(3-)', *etc.*]. Section P-65.2.1.2 of Ref. 1 prescribes 'carbonotrithioic acid', leading to the anion name 'carbonotrithioate', which will not be mistaken for an additive name.

A few examples of other functional nomenclature are also included in Table IR-8.2 (*e.g.* 'phosphoryl chloride', 'sulfuric diamide'). These particular names are well entrenched and can still be used, but this type of nomenclature is not recommended for other compounds than those shown. Again, additive and substitutive names may always be constructed, as exemplified in the Table.

IR-8.7 REFERENCES

1. **New Blue Book.**
2. *Nomenclature of Inorganic Chemistry, Recommendations 1990*, Blackwell Scientific Publications, Oxford, 1990.
3. *Nomenclature of Inorganic Chemistry II, Recommendations 2000*, Royal Society of Chemistry, 2001.
4. *IUPAC Nomenclature of Inorganic Chemistry, Second Edition, Definitive Rules 1970*, Butterworths, London, 1971.

IUPAC Provisional Recommendations