

# IR-5 Compositional Nomenclature and Overview of Names of Ions and Radicals (Draft March 2004)

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## IR-5.1 INTRODUCTION

Compositional nomenclature is formally based on composition, not structure, and may thus be the (only) choice if little or no structural information is available or a minimum of structural information is to be conveyed.

The simplest type of compositional name is a *stoichiometric* name, which is just a reflection of the empirical formula (Section IR-4.2.1) or the molecular formula (Section IR-4.2.2) of

the compound. In stoichiometric names, proportions of constituent elements may be indicated in several ways, using numerical prefixes, oxidation numbers or charge numbers.

In some cases, a compound may be viewed as composed of constituents that may themselves be given names of any of several types (including stoichiometric names), and the overall name of the compound is then assembled from the names of the constituents so as to indicate the proportions of the constituents. One category of such compositional names is *generalised stoichiometric* (see Section IR-5.4) in which the various parts may themselves be names of mono- and polyatomic ions. For this reason, Section IR-5.3, devoted to the naming of ions, is included. Another category consists of the names devised for *addition compounds* which have a format of their own, described in Section IR-5.5.

## IR-5.2 STOICHIOMETRIC NAMES OF ELEMENTS AND NEUTRAL BINARY COMPOUNDS

A purely stoichiometric name carries no information about the structure of the compound.

This section deals with stoichiometric names of neutral compounds. Stoichiometric names of ions are described in Section IR-5.3.

In the simplest case, the species to be named consists of only one element, and the name is formed by adding the relevant multiplicative prefix to the element name (*e.g.* S<sub>8</sub>, octasulfur). This case is dealt with more fully in Sections IR-3.4.2 and IR-3.5.2.

When constructing a stoichiometric name for a binary compound, one element is designated as the electropositive constituent and the other the electronegative constituent. The electropositive constituent is *by convention* the element that occurs last in the sequence of Table VI\* (except that oxygen is placed between chlorine and fluorine) and its name is the unmodified element name (Table I). The name of the electronegative constituent is constructed by modifying the element name with the ending 'ide', as explained in detail for monoatomic anions in Section IR-5.3.3.2. All element names thus modified with the 'ide' ending are given in Table IX.

The stoichiometric name of the compound is then formed by combining the name of the electropositive constituent, cited first, with that of the electronegative constituent, both suitably qualified by any necessary multiplicative prefixes ('mono', 'di', 'tri', 'tetra', 'penta', *etc.*, given in Table IV). The numerical prefixes precede the names they multiply, and are joined directly to them without spaces or hyphens. The final vowels of numerical prefixes should not be elided

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

(although monoxide, rather than monooxide, is an allowed exception through general use). The two parts of the name are separated by a space.

Stoichiometric names may correspond to the empirical formula or to a molecular formula different from the empirical formula (compare Examples 3 and 4 below).

*Examples:*

- |     |                                 |   |
|-----|---------------------------------|---|
| 1.  | HCl                             | hydrogen chloride   |
| 2.  | NO                              | nitrogen oxide, or nitrogen monooxide, or nitrogen monoxide |
| 3.  | NO <sub>2</sub>                 | nitrogen dioxide  |
| 4.  | N <sub>2</sub> O <sub>4</sub>   | dinitrogen tetroxide  |
| 5.  | Cl <sub>2</sub> O               | dichlorine oxide  |
| 6.  | ClO <sub>2</sub>                | chlorine dioxide  |
| 7.  | Fe <sub>3</sub> O <sub>4</sub>  | triiron tetraoxide  |
| 8.  | SiC                             | silicon carbide   |
| 9.  | SiCl <sub>4</sub>               | silicon tetrachloride                                       |
| 10. | Ca <sub>3</sub> P <sub>2</sub>  | tricalcium diphosphide, or calcium phosphide                |
| 11. | NiSn                            | nickel stannide   |
| 12. | Cu <sub>5</sub> Zn <sub>8</sub> | pentacopper octazincide                                     |
| 13. | Cr <sub>23</sub> C <sub>6</sub> | tricosachromium hexacarbide                                 |

Multiplicative prefixes need not be used in binary names if there is no ambiguity about the stoichiometry of the compound (such as in Example 10 above). The prefix 'mono' is, strictly speaking, superfluous and is only needed for emphasizing stoichiometry when discussing compositionally related substances, such as Examples 2, 3 and 4 above.

Alternatively, proportions of constituents may be indicated by using oxidation numbers or charge numbers (Section IR-5.4.2).

For compounds containing more than two elements, further conventions are required to form a compositional name (see Sections IR-5.4 and IR-5.5).

### IR-5.3 NAMES OF IONS

#### IR-5.3.1 **General**

The charges of the atoms need not be specified in a stoichiometric name. In many cases, however, atoms or groups of atoms are known to carry a particular charge. Within compositional nomenclature, the name of a compound can include the names of individual

such ions constructed as stoichiometric names or according to other principles, as described below.

## IR-5.3.2 Cations

### IR-5.3.2.1 *General*

A cation is a monoatomic or polyatomic species having one or more positive charges. The charge on a cation can be indicated in names and formulae by using the charge number or, in the case of additively named cations, by the oxidation number(s) of the central atom or atoms. Oxidation and charge numbers are discussed in Section IR-5.4.2.2.

### IR-5.3.2.2 *Monoatomic cations*

The name of a monoatomic cation is that of the element with an appropriate charge number appended in parentheses. Unpaired electrons in monoatomic cations may be indicated using a radical dot, *i.e.* a centred dot placed in parentheses after the name, with a numerical prefix if necessary.

*Examples:*

1. Na<sup>+</sup> sodium(1+)
2. Cr<sup>3+</sup> chromium(3+)
3. Cu<sup>+</sup> copper(1+)
4. Cu<sup>2+</sup> copper(2+)
5. I<sup>+</sup> iodine(1+)
6. H<sup>+</sup> hydrogen(1+), hydron
7. <sup>1</sup>H<sup>+</sup> protium(1+), proton
8. <sup>2</sup>H<sup>+</sup> deuterium(1+), deuteron
9. <sup>3</sup>H<sup>+</sup> tritium(1+), triton
10. He<sup>•+</sup> helium(•1+)
11. O<sup>•+</sup> oxygen(•1+)

The names of the hydrogen isotopes are discussed in Section IR-3.3.2.

### IR-5.3.2.3 *Homopolyatomic cations*

Homopolyatomic cations are named by adding the charge number to the stoichiometric name of the corresponding neutral species, *i.e.* the element name with the appropriate numerical prefix. A radical dot or radical dots may be added to indicate the presence of unpaired electrons.

*Examples:*

1.  $\text{O}_2^+$  or  $\text{O}_2^{\bullet+}$  dioxygen(1+) or dioxygen( $\bullet$ 1+)
2.  $\text{S}_4^{2+}$  tetrasulfur(2+)
3.  $\text{Hg}_2^{2+}$  dimercury(2+)
4.  $\text{Bi}_5^{4+}$  pentabismuth(4+)
5.  $\text{H}_3^+$  trihydrogen(1+)

IR-5.3.2.4 *Heteropolyatomic cations*

Heteropolyatomic cations are usually named either substitutively (see Section IR-6.4) or additively (see Chapter IR-7). Substitutive names do not require a charge number, because the name itself implies the charge (Examples 2 and 4 below). A radical dot or radical dots may be added to an additive name to indicate the presence of unpaired electrons.

A few cations have established and still allowed non-systematic names.

*Examples:*

1.  $\text{NH}_4^+$  azanium (substitutive), or ammonium (allowed non-systematic)
2.  $\text{H}_3\text{O}^+$  oxidanium (substitutive), or oxonium (allowed non-systematic)
3.  $\text{PH}_4^+$  phosphanium (substitutive)
4.  $\text{H}_4\text{O}^{2+}$  oxidanediium (substitutive)
5.  $\text{SbF}_4^+$  tetrafluorostibanium (substitutive), or tetrafluoridoantimony(1+) or tetrafluoridoantimony(V) (both additive)
6.  $\text{BH}_3^{\bullet+}$  boraniumyl (substitutive) or trihydridoboron( $\bullet$ 1+) (additive)

More examples are given in Table IX.

IR-5.3.3 **Anions**IR-5.3.3.1 *Overview*

An anion is a monoatomic or polyatomic species having one or more negative charges. The charge on an anion can be indicated in the name by using the charge number or, in the case of an additively named anion, by the oxidation number(s) of the central atom or atoms. Oxidation and charge numbers are discussed in Section IR-5.4.2.2.

The endings in anion names are 'ide' (monoatomic or homopolyatomic species, heteropolyatomic species named from the parent hydride), 'ate' (heteropolyatomic species named additively), and 'ite' (used in a few names which are still allowed but do not derive from current systematic nomenclature). When there is no ambiguity, the charge number may be omitted, as in Example 1 below. Parent hydride-based names do not carry charge numbers, because the name itself implies the charge (Examples 3 and 4 below).

*Examples:*

- |    |                        |   |
|----|------------------------|---|
| 1. | $\text{Cl}^-$          | chloride(1-), or chloride                                 |
| 2. | $\text{S}_2^{2-}$      | disulfide(2-)   |
| 3. | $\text{PH}_2^-$        | phosphanide   |
| 4. | $\text{PH}^{2-}$       | phosphanediide  |
| 5. | $[\text{CoCl}_4]^{2-}$ | tetrachloridocobaltate(2-), or tetrachloridocobaltate(II) |
| 6. | $\text{NO}_2^-$        | dioxidonitrate(1-), or nitrite                            |

#### IR-5.3.3.2 Monoatomic anions

The name of a monoatomic anion is the element name (Table I) modified so as to carry the anion designator 'ide', either formed by replacing the ending of the element name ('en', 'ese', 'ic', 'ine', 'ium', 'ogen', 'on', 'orus', 'um', 'ur', 'y', or 'ygen') by 'ide' or by directly adding 'ide' as an ending to the element name.

*Examples:*

1. chlorine, chloride
2. carbon, carbide
3. xenon, xenonide
4. tungsten, tungstide
5. bismuth, bismuthide

In one case, an abbreviated name has to be chosen: germanium, germide. The systematic name 'germanide' designates the anion  $\text{GeH}_3^-$ .

Some names of monoatomic anions are based on the root of the Latin element names. In these the ending 'um' or 'ium' is replaced by 'ide'.

*Examples:*

6. silver, argentum, argentide
7. gold, aurum, auride
8. copper, cuprum, cupride

9. iron, ferrum, ferride
10. lead, plumbum, plumbide
11. tin, stannum, stannide
12. sodium, natrium, natride
13. potassium, kalium, kalide

All element names thus modified are included in Table IX.

Charge numbers and radical dots may be added as appropriate to specify the anion fully.

*Examples:*

14.  $\text{O}^{2-}$  oxide(2-), or oxide
15.  $\text{O}^{\bullet-}$  oxide( $\bullet$ 1-)
16.  $\text{N}^{3-}$  nitride(3-), or nitride

#### IR-5.3.3.3 Homopolyatomic anions

Homopolyatomic anions are named by adding the charge number to the stoichiometric name of the corresponding neutral species, *i.e.* the element name with the appropriate numerical prefix. Again, a radical dot or dots may be added as appropriate.

In a few cases, non-systematic names are still allowed alternatives.

*Examples:*

		<i>Systematic name</i>	<i>Alternative name</i>
1.	$\text{O}_2^-$ or $\text{O}_2^{\bullet-}$	dioxide(1-) or dioxide( $\bullet$ 1-)	superoxide
2.	$\text{O}_2^{2-}$	dioxide(2-)	peroxide
3.	$\text{O}_3^-$	trioxide(1-)	ozonide
4.	$\text{I}_3^-$	triiodide(1-)	
5.	$\text{Cl}_2^{\bullet-}$	dichloride( $\bullet$ 1-)	
6.	$\text{C}_2^{2-}$	dicarbide(2-)	acetylide
7.	$\text{N}_3^-$	trinitride(1-)	azide
8.	$\text{S}_2^{2-}$	disulfide(2-)	
9.	$\text{Sn}_5^{2-}$	pentastannide(2-)	
10.	$\text{Pb}_9^{4-}$	nonaplumbide(4-)	

In some cases, homopolyatomic anions may be considered as derived from a parent hydride by removal of hydrons (see Section IR-6.4).

*Examples:*

- |     |                   |                |
|-----|-------------------|----------------|
| 10. | $\text{O}_2^{2-}$ | dioxidanediide |
| 11. | $\text{S}_2^{2-}$ | disulfanediide |

#### IR-5.3.3.4 *Heteropolyatomic anions*

Heteropolyatomic anions are usually named either substitutively (see Section IR-6.4.4) or additively (see Chapter IR-7 and Section IR-9.2.2). A radical dot, or dots, may be added to additive names to indicate the presence of unpaired electron(s).

A few heteropolyatomic anions have established and still allowed non-systematic names.

*Examples:*

- |     |                                  |  |
|-----|----------------------------------|--|
| 1.  | $\text{NH}_2^-$                  | azanide (substitutive), dihydridonitrate(1 <sup>-</sup> ) (additive), or amide (allowed non-systematic)                |
| 2.  | $\text{GeH}_3^-$                 | germanide (substitutive), or trihydridogermanate(1 <sup>-</sup> ) (additive)   |
| 3.  | $\text{HS}^-$                    | sulfanide (substitutive), or hydridosulfate(1 <sup>-</sup> ) (additive)  |
| 4.  | $\text{H}_3\text{S}^-$           | sulfanuide or $\lambda^4$ -sulfanide (both substitutive), or trihydridosulfate(1 <sup>-</sup> ) (additive)             |
| 5.  | $\text{H}_2\text{S}^{\bullet -}$ | sulfanuidyl or $\lambda^4$ -sulfanidyl (both substitutive), or dihydridosulfate( $\bullet$ 1 <sup>-</sup> ) (additive) |
| 6.  | $\text{SO}_3^{2-}$               | trioxidosulfate(2 <sup>-</sup> ) (additive), or sulfite (allowed non-systematic)                                       |
| 7.  | $\text{ClO}^-$                   | oxidochlorate(1 <sup>-</sup> ) (additive), or hypochlorite (allowed non-systematic)                                    |
| 8.  | $\text{ClO}_3^-$                 | trioxidochlorate(1 <sup>-</sup> ) (additive), or chlorate (allowed non-systematic)                                     |
| 9.  | $[\text{PF}_6]^-$                | hexafluoro- $\lambda^5$ -phosphanuide (substitutive), or hexafluoridophosphate(1 <sup>-</sup> ) (additive)             |
| 10. | $[\text{CuCl}_4]^{2-}$           | tetrachloridocuprate(II) (additive)  |
| 11. | $[\text{Fe}(\text{CO})_4]^{2-}$  | tetracarbonylferrate(-II) (additive)   |

All allowed, but not fully systematic, anion names are given in Table IX.



Note that in Ref. 1, radical anions consisting of only hydrogen and one other element were named additively using the ending 'ide' rather than the ending 'ate' (*e.g.* Example 5 above). Making this exception to the general system of additive nomenclature for these particular cases is now discouraged.

When one or more hydron(s) are attached to an anion at an unknown position(s), or at a position(s) which one cannot or does not wish to specify, a 'hydrogen name' (see Section IR-8.4) may be used. Such names may also be used for simpler compounds, such as partially dehydrogenated oxoacids. Certain of these names have accepted abbreviated forms, such as hydrogencarbonate, dihydrogenphosphate, *etc.* All such accepted abbreviated names are given in Section IR-8.5.

*Examples:*

- |     |                               |  |
|-----|-------------------------------|--|
| 12. | $\text{HMo}_6\text{O}_{19}^-$ | hydrogen(nonadecaoxidohexamolybdate)(1-)                       |
| 13. | $\text{HCO}_3^-$              | hydrogen(trioxidocarbonate)(1-), or hydrogencarbonate          |
| 14. | $\text{H}_2\text{PO}_4^-$     | dihydrogen(tetraoxidophosphate)(1-),<br>or dihydrogenphosphate |

#### IR-5.4 GENERALISED STOICHIOMETRIC NAMES

##### IR-5.4.1 **Electropositive and electronegative constituents; order of citation**

The constituents of the compound to be named are divided into formally electropositive and formally electronegative constituents. There must be at least one electropositive and one electronegative constituent. Cations are electropositive and anions electronegative, by definition. Electropositive elements occur later in Table VI than electronegative elements, except that oxygen is placed between chlorine and fluorine by custom.

In principle, the division into electropositive and electronegative constituents is arbitrary if the compound contains more than two elements. In practice, however, there is often no problem in deciding where the division lies.

The names of the electropositive constituents precede those of the electronegative constituents in the overall name. The order of citation is alphabetical within each class of constituents (multiplicative prefixes being ignored), except that hydrogen is always cited last among electropositive constituents if actually classified as an electropositive constituent.

This principle for constructing generalised stoichiometric names parallels the principle for constructing 'generalised salt formulae' in Section IR-4.4.3.4. However, the order of citation in

a generalised stoichiometric name is not necessarily the same as the order of symbols in the corresponding generalised salt formula, as is seen from Examples 5 and 7 below.

The following generalised stoichiometric names, based only on single-element constituents, do not carry information about the structure.

*Examples:*

- |    |  |   |
|----|--|---|
| 1. | IBr  | iodine bromide  |
| 2. | PBrClI   | phosphorus bromide chloride iodide  |
| 3. | ArHF or ArFH   | argon hydrogen fluoride, or argon fluoride hydride                            |
| 4. | ClOF or ClFO   | chlorine oxygen fluoride or chlorine fluoride oxide                           |
| 5. | CuK <sub>5</sub> Sb <sub>2</sub> or K <sub>5</sub> CuSb <sub>2</sub> | copper pentapotassium diantimonide, or<br>pentapotassium cupride diantimonide |

Note from these examples that the order of any two elements in the name depends on the arbitrary division of elements into electropositive and electronegative constituents. (The same applies to the order of the element symbols in the formulae as illustrated in Section IR-4.4.3.4). Additive names representing the actual structure of the compounds in Examples 3 and 4 (FArH and FCIO, respectively) are given in Section IR-7.2.

In some cases, the use of substitutive or additive nomenclature for naming an ion is not possible or desirable because of the lack of structural information. In such cases, it may be best to give a stoichiometric name and add the charge number. Parentheses are needed to make it clear that the charge number is associated with the entire compound.

*Example:*

- |    |   |                          |
|----|---|--------------------------|
| 6. | Cl <sub>2</sub> O <sub>2</sub> <sup>+</sup> | (dichlorine dioxide)(1+) |
|----|---|--------------------------|

However, when names of polyatomic ions occur as constituents in a generalised stoichiometric name, a certain amount of structural information is often implied by the name.

*Example:*

- |    |                                       |                                   |
|----|---------------------------------------|-----------------------------------|
| 7. | NaNH <sub>4</sub> [HPO <sub>4</sub> ] | ammonium sodium hydrogenphosphate |
|----|---------------------------------------|-----------------------------------|

## IR-5.4.2 Indication of proportions of constituents

### IR-5.4.2.1 Use of multiplicative prefixes

The proportions of the constituents, be they monoatomic or polyatomic, may be indicated in generalised stoichiometric names by numerical prefixes, as was the case for the constituents of binary compounds (Section IR-5.2).

*Examples:*

1.  $\text{Na}_2\text{CO}_3$  disodium trioxidocarbonate, or sodium carbonate
2.  $\text{K}_4[\text{Fe}(\text{CN})_6]$  tetrapotassium hexacyanidoferrate
3.  $\text{PCl}_3\text{O}$  phosphorus trichloride oxide
4.  $\text{KMgCl}_3$  magnesium potassium trichloride

When the name of the constituent itself starts with a multiplicative prefix (as in disulfate, dichromate, triphosphate, tetraborate, *etc.*), or when ambiguity could otherwise arise, the alternative multiplicative prefixes 'bis', 'tris', 'tetrakis', 'pentakis', *etc.* (Table IV) are used and the name of the group acted upon by the alternative prefix is placed in parentheses.

*Examples:*

5.  $\text{Ca}(\text{NO}_3)_2$  calcium bis(trioxidonitrate), or calcium nitrate
6.  $(\text{UO}_2)_2\text{SO}_4$  bis(dioxidouranium) tetraoxidosulfate
7.  $\text{Ba}[\text{BrF}_4]_2$  barium bis(tetrafluoridobromate)
8.  $\text{U}(\text{S}_2\text{O}_7)_2$  uranium bis(disulfate)
9.  $\text{Ca}_3(\text{PO}_4)_2$  tricalcium bis(phosphate)
10.  $\text{Ca}_2\text{P}_2\text{O}_7$  calcium diphosphate
11.  $\text{Ca}(\text{HCO}_3)_2$  calcium bis(hydrogencarbonate)

#### IR-5.4.2.2 *Use of charge and oxidation numbers*

It is possible to provide information on the proportions of the constituents in names by using one of two other devices: the charge number, which designates ionic charge, and the oxidation number, which designates oxidation state. In nomenclature, the use of the charge number is preferred as the determination of the oxidation number is sometimes ambiguous and subjective. It is therefore advisable to use oxidation numbers only when there is no uncertainty about their assignment.

The *charge number* is a number whose magnitude is the ionic charge. It is written in parentheses immediately after the name of an ion, without a space. The charge is written in arabic numerals, followed by the sign of the charge. Note that unity (1) is always indicated, unlike in superscript charge designations (which are used in formulae). No charge number is used after the name of a neutral species.

*Examples:*

- |    |  |                                       |
|----|--|---------------------------------------|
| 1. | FeSO <sub>4</sub>  | iron(2+) sulfate                      |
| 2. | Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>          | iron(3+) sulfate                      |
| 3. | (UO <sub>2</sub> ) <sub>2</sub> SO <sub>4</sub>          | dioxidouranium(1+) sulfate            |
| 4. | UO <sub>2</sub> SO <sub>4</sub>                          | dioxidouranium(2+) sulfate            |
| 5. | K <sub>4</sub> [Fe(CN) <sub>6</sub> ]                    | potassium hexacyanidoferrate(4-)      |
| 6. | [Co(NH <sub>3</sub> ) <sub>6</sub> ]Cl(SO <sub>4</sub> ) | hexaamminecobalt(3+) chloride sulfate |

The *oxidation number* (see Sections IR-4.6.1 and IR-9.1.2.8) of an element is indicated by a Roman numeral placed in parentheses immediately following the name (modified by the ending 'ate' if necessary) of the element to which it refers. The oxidation number may be positive, negative or zero (represented by the numeral 0). An oxidation number is always non-negative unless the minus sign is explicitly used (the positive sign is never used). Non-integral oxidation numbers are not used for nomenclature purposes.

*Example:*

- |    |                          |                                   |
|----|--------------------------|-----------------------------------|
| 7. | PCl <sub>5</sub>         | phosphorus(V) chloride            |
| 8. | Na[Mn(CO) <sub>5</sub> ] | sodium pentacarbonylmanganate(-I) |
| 9. | [Fe(CO) <sub>5</sub> ]   | pentacarbonyliron(0)              |

Several conventions are observed for inferring oxidation numbers, the use of which is particularly common in the names of compounds of transition elements. Hydrogen is considered positive (oxidation number I) in combination with non-metallic elements and negative (oxidation number -I) in combination with metallic elements. Organic groups combined with metal atoms are treated sometimes as anions (for example, a methyl ligand is usually considered to be a methanide ion, CH<sub>3</sub><sup>-</sup>), sometimes as neutral (*e.g.* carbon monoxide). Bonds between atoms of the same species make no contribution to oxidation number.

*Examples:*

- |     |   |                            |
|-----|---|----------------------------|
| 10. | N <sub>2</sub> O                                | nitrogen(I) oxide          |
| 11. | NO <sub>2</sub>                                 | nitrogen(IV) oxide         |
| 12. | Fe <sub>3</sub> O <sub>4</sub>                  | iron(II) diiron(III) oxide |
| 13. | MnO <sub>2</sub>                                | manganese(IV) oxide        |
| 14. | CO  | carbon(II) oxide           |
| 15. | FeSO <sub>4</sub>                               | iron(II) sulfate           |
| 16. | Fe <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub> | iron(III) sulfate          |
| 17. | SF <sub>6</sub>                                 | sulfur(VI) fluoride        |
| 18. | (UO <sub>2</sub> ) <sub>2</sub> SO <sub>4</sub> | dioxidouranium(V) sulfate  |

- |     |  |   |
|-----|--|---|
| 19. | $\text{UO}_2\text{SO}_4$                           | dioxidouranium(VI) sulfate  |
| 20. | $\text{K}_4[\text{Fe}(\text{CN})_6]$               | potassium hexacyanidoferrate(II), or<br>potassium hexacyanidoferrate(4-)            |
| 21. | $\text{K}_4[\text{Ni}(\text{CN})_4]$               | potassium tetracyanidonickelate(0), or<br>potassium tetracyanidonickelate(4-)       |
| 22. | $\text{Na}_2[\text{Fe}(\text{CO})_4]$              | sodium tetracarbonylferrate(-II), or<br>sodium tetracarbonylferrate(2-)             |
| 23. | $[\text{Co}(\text{NH}_3)_6]\text{Cl}(\text{SO}_4)$ | hexaamminecobalt(III) chloride sulfate, or<br>hexaamminecobalt(3+) chloride sulfate |
| 24. | $\text{Fe}_4[\text{Fe}(\text{CN})_6]_3$            | iron(III) hexacyanidoferrate(II), or<br>iron(3+) hexacyanidoferrate(4-)             |

Note that oxidation numbers are no longer recommended when naming homopolyatomic ions. This is to avoid ambiguity. Oxidation numbers refer to the individual atoms of the element in question, even if they are appended to a name containing a multiplicative prefix, *cf.* Example 12 above. To conform to this practice, dimercury(2+) (see Section IR-5.3.2.3) would have to be named dimercury(I); dioxide(2-) (see Section IR-5.3.3.3) would be dioxide(-I); and ions such as pentabismuth(4+) (see Section IR-5.3.2.3) and dioxide(1-) (see Section IR-5.3.3.3), with fractional formal oxidation numbers, could not be named at all.

#### IR-5.4.2.3 *Multiple monoatomic constituents vs. homopolyatomic constituents*

Care should be taken to distinguish between multiple monoatomic constituents and polyatomic constituents. This distinction is often not apparent from the formula, but is tacitly implied.

*Examples:*

- |    |                         |  |
|----|-------------------------|--|
| 1. | $\text{TlI}_3$          | thallium tris(iodide), or thallium(III) iodide, or<br>thallium(3+) iodide      |
| 2. | $\text{Tl}(\text{I}_3)$ | thallium (triiodide), or thallium triiodide(1-),<br>or thallium(I) (triiodide) |

Both compounds in Examples 1 and 2 have the overall formula  $\text{TlI}_3$  and both could be named by the simple stoichiometric name thallium triiodide. However, it is possible – and usually desirable – to convey more information in the name.

The compound in Example 1 consists of iodide,  $\text{I}^-$ , and thallium, in the proportion 3:1, whereas the compound in Example 2 consists of triiodide(1-),  $\text{I}_3^-$ , and thallium in the proportion 1:1. In the simple stoichiometric name for the first compound, then, the numerical

prefix 'tris' is used to make it completely clear that three iodide ions are involved rather than one triiodide ion. The alternative names use the oxidation number III for thallium and the charge number 3+, respectively, to convey the proportions of the constituents.

In the first name in Example 2, the parentheses indicate that the electronegative constituent is a homopolyatomic entity. The second name is even more informative in giving the charge of the anion, and this can also be indicated indirectly by using the oxidation number for thallium as shown in the third name.

*Examples:*

- |    |                          |   |
|----|--------------------------|---|
| 3. | $\text{HgCl}_2$          | mercury dichloride, or mercury(II) chloride,<br>or mercury(2+) chloride       |
| 4. | $\text{Hg}_2\text{Cl}_2$ | dimercury dichloride, or (dimercury) dichloride,<br>or dimercury(2+) chloride |

In Example 4, the first name is purely stoichiometric, whereas the second name contains more information in indicating that the compound contains a homodiatom cation. In the last name, where the charge of the dication is specified, the prefix 'di' for 'chloride' is not necessary.

*Examples:*

- |    |                         |   |
|----|-------------------------|---|
| 5. | $\text{Na}_2\text{S}_3$ | disodium (trisulfide)<br>(this indicates the presence of the polyatomic anion),<br>or sodium trisulfide(2-)<br>(with the charge on the anion indicated, the numerical prefix<br>on the cation is not necessary) |
| 6. | $\text{Fe}_2\text{S}_3$ | diiron tris(sulfide), or iron(III) sulfide  |

Salts which contain anions that are composed of  $\text{S}_n^{2-}$  chains, as well as those containing several  $\text{S}^{2-}$  anions, are both referred to as 'polysulfides' but, as demonstrated, names may be given that provide a distinction between these cases.

*Examples:*

- |     |                        |   |
|-----|------------------------|---|
| 7.  | $\text{K}_2\text{O}$   | dipotassium oxide                               |
| 8.  | $\text{K}_2\text{O}_2$ | dipotassium (dioxide), or potassium dioxide(2-) |
| 9.  | $\text{KO}_2$          | potassium (dioxide), or potassium dioxide(1-)   |
| 10. | $\text{KO}_3$          | potassium (trioxide), or potassium trioxide(1-) |

Clearly, a simple stoichiometric name like 'potassium dioxide', although strictly speaking unambiguous (referring to the compound in Example 9), could easily be misinterpreted. In other cases, based on chemical knowledge, there is no chance of misinterpretation in practice, and the simple stoichiometric name will most often be used, as in Examples 11 and 12 below.

*Examples:*

- |     |                |   |
|-----|----------------|---|
| 11  | $\text{BaO}_2$ | barium dioxide (simple stoichiometric name), or<br>barium (dioxide), or barium dioxide(2 <sup>-</sup> ) (specifies dianion)                                 |
| 12. | $\text{MnO}_2$ | manganese dioxide (simple stoichiometric name), or<br>manganese bis(oxide), or manganese(IV) oxide<br>(this specifies two oxide ions rather than a dianion) |

## IR-5.5 NAMES OF ADDITION COMPOUNDS

The term *addition compounds* covers donor-acceptor complexes and a variety of lattice compounds. The method described here, however, is relevant not just to such compounds, but also to multiple salts and to certain compounds of uncertain structure.

The names of the individual components of such a generalised addition compound are constructed by using an appropriate nomenclature system, whether compositional, substitutive or additive. The overall name of the compound is then formed by connecting the names of the components by 'em' dashes; the proportions of the components are indicated after the name by a stoichiometric descriptor consisting of arabic numerals separated by a solidus. The descriptor, in parentheses, is separated from the compound name by a space. The sequence of names of the individual components is the same as the sequence in the formula (Section IR-4.4.3.5). In addition compounds, the name of  $\text{H}_2\text{O}$  is 'water'. The term 'hydrate' has a specific meaning, *i.e.* a compound containing water of crystallization bound in an unspecified way.

*Examples:*

- |    |   |  |
|----|---|--|
| 1. | $\text{BF}_3 \cdot 2\text{H}_2\text{O}$   | boron trifluoride—water (1/2)                      |
| 2. | $8\text{Kr} \cdot 46\text{H}_2\text{O}$   | krypton—water (8/46)                               |
| 3. | $3\text{CdSO}_4 \cdot 8\text{H}_2\text{O}$  | cadmium sulfate—water (3/8)                        |
| 4. | $\text{Al}_2(\text{SO}_4)_3 \cdot \text{K}_2\text{SO}_4 \cdot 24\text{H}_2\text{O}$ | aluminium sulfate—potassium sulfate—water (1/1/24) |
| 5. | $\text{CaCl}_2 \cdot 8\text{NH}_3$  | calcium chloride—ammonia (1/8)                     |
| 6. | $\text{AlCl}_3 \cdot 4\text{EtOH}$  | aluminium chloride—ethanol (1/4)                   |
| 7. | $\text{BiCl}_3 \cdot 3\text{PCl}_5$   | bismuth(III) chloride—phosphorus(V) chloride (1/3) |
| 8. | $2\text{Na}_2\text{CO}_3 \cdot 3\text{H}_2\text{O}_2$                               | sodium carbonate—hydrogen peroxide (2/3)           |

9.  $\text{Co}_2\text{O}_3 \cdot n\text{H}_2\text{O}$  cobalt(III) oxide—water (1/*n*)

IR-5.6 FINAL REMARKS

Compositional names are either of the stoichiometric type (which, furthermore, are of the binary type except in the case of homoatomic species) or of the addition compound type. Compositional nomenclature is used if little or no structural information is to be conveyed by the name. However, substitutive or additive nomenclature may be used to indicate the structure of constituents of a compound that is named overall by compositional nomenclature. Substitutive nomenclature is described in Chapter IR-6 and additive nomenclature in Chapters IR-7, IR-8, and IR-9.

IR-5.7 REFERENCES

1. Names for Inorganic Radicals, *Pure Appl. Chem.*, **72**, 437 (2000).

IUPAC Provisional Recommendations