

## Inorganic Chemistry Nomenclature: Newsletter 1990

### IUPAC Commission on Inorganic Chemistry Nomenclature

#### Introduction

Nomenclature can be occasionally confusing, especially when different authors use different terms for the same compounds. It is particularly annoying when an author uses two different nomenclatures in the same paper. One of the reasons for CNIC to publish Newsletters on Nomenclature is to raise issues and to help avoiding misunderstandings about inorganic nomenclature, with the hope of contributing to better understanding and communication. The Commission on Nomenclature of Inorganic Chemistry (CNIC) has, as its ultimate task, to devise recommendations to the chemical society, according to which chemical structures can be unambiguously and uniquely converted to names and vice versa. To help CNIC in this communication process and encourage scientists to contact the commission about problems and to make suggestions, a biannual Newsletter is a useful medium.

In this Newsletter reports are given about ongoing projects, and in addition a few items of actual interest will be discussed. Readers are invited to write to the CNIC chairman (Professor A. M. Sargeson, Australian National University, Canberra, Australia), or its secretary (see below), about problems in Nomenclature of Inorganic Chemistry.

#### IUPAC–CNIC 1990 Nomenclature Recommendations (The New Red Book)

After a 12 year period of preparation and consultation with experts in several subdisciplines, the 3rd edition of the so-called New Red Book appeared at the beginning of 1990. It is available both in a hard cover and in a cheaper soft cover [1]. Summaries of the several chapters were published in the previous Newsletter (1987) [2].

#### *Nomenclature of polyanions*

In the previous Newsletter it was announced that a document on polyanions was in press. This document has now been published [3], and describes how systematic names can be derived for the great variety of polynuclear molybdates and tungstates,

and many derivatives. Even structural information can be derived from the names for these anions.

#### *Periodic table*

As indicated before the New Red Book contains 3 different periodic tables, i.e. 8 columns, 18 columns and 32 columns. When the 18 column table is used, CNIC now recommends that authors should use the numbering 1–18 for numbering the columns in scientific communications.

#### *Names of certain neutral and anionic ligands*

About 20 years ago it was decided that negative ligands should have names ending in -o, like chloro, bromo, imidazolato, oxo, hydroxo, superoxido, etc. Only certain organic radicals as anionic ligands may remain unchanged like methyl, phenyl. Small neutral molecules have names like aqua ( $\text{H}_2\text{O}$ ) and *not* aquo. The name for ligated ammonia ( $\text{NH}_3$ ) has two 'm's (ammine), while coordinated organic amines are spelled with a single 'm', e.g. methylamine. Bound carbon monoxide is carbonyl (CO). Neutral ligands without special names keep their names unchanged, but are used in enclosing marks when coordinated, e.g. (dinitrogen), (dihydrogen), (methanol), etc.

#### *Trivial names for certain ions*

For a very long time  $\text{Fe}^{2+}$ ,  $\text{Fe}^{3+}$  and  $\text{Cu}^+$ ,  $\text{Cu}^{2+}$  have been named ferrous, ferric and cuprous, cupric, respectively. However, since Fe(IV) and Cu(III) have also been found in many compounds CNIC suggests iron(II), Fe(II); iron(III), Fe(III); copper(I), Cu(I); copper(II), Cu(II), etc. be used.

#### *Use of -ate and -and suffixes*

Originating from the words ligand and chelate users in the field have been designing ligand group names, like cheland, cryptand, podand, coronand, sepulchrand etc. to describe certain chelating ligands. In addition the resulting metal complexes have been indicated as chelates, cryptates, podates, coronates and sepulchrates. Users of these terminology should realize that these names do not necessarily suggest a negative charge of the complexes (like e.g. tetrachloroferrate(II) for  $\text{FeCl}_4^{2-}$ ). Further, the term 'ligate' is only to be used as a verb, and not as a noun.

It has been observed that the terms liganding and liganded have appeared in the literature. These words have no linguistic status and the correct terms are coordinating (or ligating) and coordinated (or ligated), respectively.

#### *Charge of cations and anions*

It is now generally agreed to use only the format:  $\text{Al}^{3+}$ ,  $\text{SO}_4^{2-}$ ,  $\text{Mn}^{2+}$  etc., and *not*  $\text{Al}^{+++}$ ,  $\text{SO}_4^{-2}$ ,

$Mn^{+2}$ ,  $S^{--}$ ,  $S^-$  etc. In the case of radical ions one should register the radical dot first, followed by the charge, e.g.  $O_2^{\cdot-}$ .

#### Ligand abbreviations

It would be a great advantage in communication if all chemists and journal editors would use the same abbreviations to describe ligands. As a first step towards this situation, the New Red Book contains a list of about 90 recommended abbreviations for common and frequently used ligands. It is hoped that inorganic chemists and journals will soon use these abbreviations throughout. Guidelines for composing abbreviations are also to be found in the New Red Book, one of them being that all papers using (ligand) abbreviations should explain these at least once in the text. Eventually the list mentioned in the Red Book will be extended, based on interactions with scientists in the field. Professor S. Kirschner, Dept. of Chemistry, Wayne State University, Detroit, MI, U.S.A., is collecting new items and readers are invited to write to him about this matter. It is intended that future ligand abbreviations should also contain indications for situations where a (non-acidic) hydrogen has been lost, and to indicate the donor atom(s) in the coordinated ligand.

#### Square brackets

Coordination entities are to be placed between square brackets, as in  $[Ni(H_2O)_6](ClO_4)_2$ ; note that the  $ClO_4^-$  anion and other common oxo anions can be considered a coordination anion, but common practice allows either no enclosing marks, as in  $[Ag(NH_3)_2]NO_3$ , or parentheses where a subscript is needed.

#### Recently published documents of interest for inorganic chemists

The Commission on Physical Organic Chemistry has recently published a document [4] on the use of names for hydrogen isotopes, as neutral species and as ions. A consequence of this use is that  $H^+$  is to be named as a proton, only when  $^1H$  is meant (like in proton NMR). The names  $^2H$  = deuterium,  $^3H$  = tritium follow from this. In cases where the isotope mixture is meant, one should use hydron. This usage has been taken up throughout the New Red Book and is part of the systematization of nomenclature. Although many chemists will find this nomenclature awkward, the students learning chemistry may find it easier, more systematic and less confusing.

#### Ongoing activities

CNIC is currently working on several topics of more specialized nomenclature, for inclusion in the so-called Red Book, Part II.

Topics to be expected to be included there are:

1. Nomenclature of polyanions [3]
2. Nomenclature of nitrogen hydrides [5]
3. Nomenclature of isotopically-labelled compounds [6]
4. Graphite intercalation compounds [7]
5. Inorganic polymeric compounds [8]
6. Inorganic rings and chains [9].

At a later stage Part III, dealing with organometallic chemistry and complicated cluster compounds, is foreseen.

#### Concluding remarks

In the case of other nomenclature matters, members are free to contact any member of CNIC, whose present chairman is Professor A. M. Sargeson. The address of the present secretary is: Professor R. S. Laitinen, Department of Chemistry, University of Oulu, Linnanmaa, SF-90570 Oulu, Finland. Other titular members of CNIC are D. Coucouvanis (Ann Arbor, MI, U.S.A.), J. McCleverty (Birmingham, U.K.), M. W. G. de Bolster (Amsterdam, The Netherlands), T. E. Sloan (Columbus, OH, U.S.A.), K. Wieghardt (Bochum, F.R.G.).

#### References

- 1 G. J. Leigh (ed.), *Nomenclature of Inorganic Compounds*, Blackwell, Oxford, 1990.
- 2 Newsletter Inorganic Chemistry 1987, *Transition Met. Chem.*, 12 (1987) 278–281.
- 3 Nomenclature of polyanions, *Pure Appl. Chem.*, 59 (1988) 1529–1548.
- 4 Names for hydrogen atoms, ions or groups and for reactions involving them, *Pure Appl. Chem.*, 60 (1988) 118–119.
- 5 The nomenclature of hydrides of nitrogen and derived cations, anions and ligands, *Pure Appl. Chem.*, 54 (1982) 2545–2552.
- 6 Nomenclature of isotopically modified compounds, *Pure Appl. Chem.*, 54 (1981) 1887–1900.
- 7 Nomenclature of graphite intercalation compounds, *Pure Appl. Chem.*, 51 (1979) 1561–1571.
- 8 Nomenclature for regular single-strand and quasi-single-strand inorganic and coordination polymers, *Pure Appl. Chem.*, 57 (1985) 149–168.
- 9 Nomenclature of inorganic ring and chain compounds, *Pure Appl. Chem.*, in preparation.