

## IUPAC COMMISSION ON NOMENCLATURE OF INORGANIC CHEMISTRY NEWSLETTER 1985

### Introduction

The objective of this Newsletter is to inform the readers of this journal about ongoing activities of this commission\* and to draw attention to its recently published nomenclature documents. Chemists are invited to write about inorganic chemistry nomenclature problems to the present vice chairman:

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or to any of its members.\*

### Recently Published Documents

In addition to the book of nomenclature [1], the commission has published several documents about topics that have evolved since 1970. The recommendations that have been published from 1982 on, deal with isotopically labeled and isotopically substituted compounds [2], inorganic and coordination polymers [3] (joint activity with the Nomenclature Commission of the Macromolecular Division), and nitrogen hydrides [4]. Short summaries of these recommendations are given below.

### Isotopically Labeled and Isotopically Substituted Compounds [2]

These rules provide a general system of nomenclature for inorganic compounds whose isotopic nuclide composition deviates from that which occurs in nature. They are also suitable for designating individual isotopic molecular species. An isotopically modified organic residue occurring in an inorganic compound, such as an organic ligand in a coordination entity, is named according to the rules of the Nomenclature of Organic Chemistry.

There is one other general system in use for describing isotopically modified compounds. It is based on an extension of the principles proposed by Boughton for designating compounds containing hydrogen isotopes, and, although mainly used in the

index nomenclature of The Chemical Abstracts Service, it is found in the literature and in some chemical catalogs.

The system of nomenclature for isotopically modified inorganic compounds codified in these rules provides for recognition of various types of isotopic modification, and thus was chosen over the system based on the Boughton principles.

### Inorganic and Coordination Polymers [3]

The fundamental principles of polymer nomenclature, which were developed to provide a framework for the unambiguous systematic naming of single-strand organic polymers, are extended to embrace inorganic and coordination polymers. The structures treated are regular single-strand polymers, that is polymers comprising repeating units linked exclusively through single atoms, and regular quasi-single-strand polymers, in which each repeating unit terminates at a single atom on one side but at a plurality of atoms on the other.

The name of the polymer is the name of the constitutional repeating unit (CRU) prefixed by the terms 'poly', 'catena', or other appropriate structural indicator, the CRU in turn being named by citing, in order of appearance along the chain, of its constituent subunits, which are the largest structural fragments of the CRU that can be named according to established principles of inorganic and/or coordination nomenclature.

The document contains rules for the identification and orientation of the CRU, and it contains many examples of inorganic/coordination polymer structures together with the recommended names.

### Nitrogen Hydrides [4]

These rules apply mainly to nitrogen hydrides containing one or two nitrogen atoms. The hydrides are considered as inorganic, although many of their derivatives are organic: the rules compromise between the relevant systems of nomenclature.

The benefit of a systematic nomenclature based on the name 'azane' for  $\text{NH}_3$  and the atom name 'nitrogen' is outlined. However, due to common practice, names from 'ammonia' ( $\text{NH}_3$ ), 'hydrazine' ( $\text{N}_2\text{H}_4$ ), 'diazene' ( $\text{N}_2\text{H}_2$ ), and 'nitrogen' (N) are retained for present use. The cations derived from the nitrogen hydrides by the addition of one or two hydrogen ions

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are names using the 'ium' ending, and the anions derived by the loss of one or more hydrogen ions by the use of the 'ide' ending in the established manner. The anions resulting from the loss of all hydrogen as ions from the nitrogen hydrides are named from the atom; e.g., nitride ( $\text{N}^{3-}$ ). The problem of naming ligands  $\text{N}_n\text{H}_m$  attached to transition metal ions where the actual valence bond structure of the ligand is indeterminate has been explored. The rules recommend that  $\text{N}_n\text{H}_m$  ligands should be named as neutral molecular species where possible, otherwise as anions, zwitterions or cationic ligands in that order of priority, but not as radicals. A table of ligand names is appended.

### Ongoing Activities

Due to many new fields and to the discovery of many new types of compounds since the publication of the Red Book (1970), it was felt necessary to completely revise the Rules for Nomenclature in Inorganic Chemistry. The commission has agreed to publish a basic manual with the following contents:

1. Aims, Function, and Methods
2. Grammar
3. Elements and Symbols
4. Formulae
5. Stoichiometric Names
6. Solid State Chemistry
7. Neutral Molecular Compounds
8. Ions, Radicals, and Salts
9. Oxoacids
10. Coordination Compounds
11. Boron Compounds

In addition to this basic material, the commission intends to publish a part II, made of chapters dealing with more advanced and detailed recommendations covering more specialized fields such as those mentioned above [2, 3, 4], heteropolyanions [5] (almost completed, publication expected in 1985), organometallic compounds, inorganic rings and chains (all in preparation).

Individual chemists are encouraged to write to the commission if they would have ideas or suggestions about these topics or to include other subjects, or if they feel that a particular field is lacking accepted rules of nomenclature.

### Correspondence, Small Matters that Matter, etc.

CNIC is a unit of an international public service organization, IUPAC, and we are volunteer chemists from about the world. Since nomenclature is our responsibility, we invite your inquiries and suggestions. We can serve you best if we know your needs and opinions. At worst, we should know someone who can name your cluster – or your ligand! Of course, some people already bring us their questions.

CNIC was formed to eliminate the Tower of Chemical Babel and almost every chemist has both appreciated and despised the tedium of the systematic and proper chemical nomenclature that CNIC is obliged to generate. In this second era of the computer evolution, names, formulae, and the like are constrained by the inevitable super-literal reaction of the computer. With sympathy, but because precision and uniformity are increasingly important, we will just point out a few conventions that deserve to be observed.

1. Representatives from all over the world agreed years ago (1970) to name the coordinated water molecule 'aqua'. Please do not call it aquo!!

2. When numerical prefixes are used in naming a coordination entity, all vowels remain in the name. In technicalese: 'there is no elision of vowels'. For example  $[\text{Al}(\text{H}_2\text{O})_6]^{3+}$  is hexaaquaaluminium(3+) ion.

3. This should not seem odd but it seems to cause some problems. The formulae of the common oxoanions are not considered to be coordination formulae. Consequently, they are not enclosed in square brackets, but rather in parentheses.  $[\text{Ni}(\text{H}_2\text{O})_6](\text{ClO}_4)_2$ .

### References

- 1 International Union of Pure and Applied Chemistry, 'Nomenclature of Inorganic Chemistry (1970)', 2nd Edn., Butterworths, London, 1971.
- 2 Nomenclature of Isotopically Modified Compounds, *Pure Appl. Chem.*, 53, 1887–1900 (1981).
- 3 Nomenclature for Regular Single-Strand and Quasi-Single-Strand Inorganic and Coordination Polymers, *Pure Appl. Chem.*, 57, 149–168 (1985).
- 4 The Nomenclature of Hydrides of Nitrogen and Derived Cations, Anions, and Ligands, *Pure Appl. Chem.*, 54, 2545–2552 (1982).
- 5 Nomenclature of Heteropolyanions (1985) in preparation.