IUPAC Commission II.2 (Commission on the Nomenclature of Inorganic Chemistry, CNIC)

Chairman: Prof. **Herb D. Kaesz**
Secretary: Dr. **Ture Damhus**

Minutes of CNIC annual meeting in Dublin, August 2000

Final version, October 29, 2000

Commission members and observers present for all or part of the meeting:

Dr. **James B. Casey**
Prof. **Neil G. Connelly**
Dr. **Ture Damhus**
Prof. **Andreas Dress**
Dr. **Piroska Fodor-Csányi**
Dr. **Richard M. Hartshorn***
Dr. **Alan T. Hutton***
Prof. **Herbert D. Kaesz**
Prof. **W. H. Koppenol**
Prof. **Risto Sakari Laitinen**
Prof. **Hiroshi Nakazawa**
Dr. **Ebbe Nordlander**
Prof. **Albrecht Salzer**

***** participating for the first time in a CNIC meeting

Special guest, present on August 20:

Dr. **Janusz Wisniewski** (member of CNOC)

The main meeting took place during the days August 19-21. Those commission members who had arrived early had, in addition, a business dinner on the evening of August 18, and on August 22, the chairman, the IDCNS representative (J.B. Casey) and the secretary met to recapitulate highlights of the meeting and some of the agreed actions, one purpose being to provide Casey with a preliminary summary of the meeting to bring to the then imminent IDCNS meeting.

The facilities at Trinity College in Dublin had been made available to the Commission by Division President Sean Corish, and during the entire meeting, the Commission was greatly aided in practical matters by Dr. Yuri Gun'ko, also of Trinity College.

Formalities

With commission secretary Constantine A. Stewart not being able to extend his association with the Commission, T. Damhus had agreed to take on the secretary's responsibilities for the period until (and including) the 2001 meeting in Brisbane.

The present minutes do not reflect the chronological progression of the meeting, but rather, under each subject, highlight key arguments of the discussions and then conclusions and actions agreed upon.

Document circulation within CNIC

It was agreed at the meeting that document circulation will generally take place via E-mail, with the documents being attached as **MS Word** files *and* **.rtf** files in order to ensure widest possible accessibility. Dr. Fodor-Csányi, however, will receive documents as hard copies by ordinary mail.

Corrections should be either written clearly in the margin of a printed version of the document in question and faxed back to the person who needs them, or an E-mail should be sent in which reference is made to specific lines/paragraphs in text where changes are suggested.

The edit mode of **Word** should not be used for communicating corrections to documents, and burying comments in an E-mail-embedded version of the document is also discouraged, since it is a tedious task for the receiver to locate all comments.

Minutes 1999 (and earlier)

The minutes of the CNIC meeting in Berlin in August 1999 were approved after some revisions had been made. It was mentioned that signed hard copies of minutes from a number of years are still kept by two former secretaries (Laitinen and Koppenol) and maybe also by Stewart. The chairman will inquire at the IUPAC secretariat as to which procedures exist for archiving minutes. In the meantime, Laitinen and Koppenol will forward their collections of minutes to the present secretary.

Some confusion had arisen in relation to the document on organometallic nomenclature by A. Salzer discussed also at the Berlin meeting. Some commission members had had the impression that the document would be circulated for last comments following the Berlin meeting. As it turned out, the version handed out at the Berlin meeting with the subtitle 'IUPAC Recommendations 2000' later appeared in print [*Pure Appl. Chem.* **71** # 8 (1999) 1557-1585] with the subtitle 'IUPAC Recommendations 1999'. The chairman took the responsibility for having cut the long-lasting discussion of this document short and having forwarded it directly to *PAC* via IDCNS. Salzer further explained that at the time of publication, which was in early 2000, *PAC* had been so far behind that the next issue to appear was to be the August 1999 issue. Since it would look strange to have recommendations named 'Recommendations 2000' appear in a 1999 issue of the journal, he had decided to change '2000' back to '1999'.

Status on Red Book II (N. Connelly)

Connelly explained that the contract between IUPAC and The Royal Society of Chemistry about publication of Red Book II had just been signed. Alan McNaught is involved in the project from the RSC. Some of the drawings need to be improved, but Jon McCleverty has arranged that Connelly will work at this together with RSC staff. Otherwise, no further revisions of the manuscript are envisaged. According to earlier agreement, P. Fodor-Csányi will receive proofs of RBII when the time comes.

Connelly will forward the table of contents of RB II to the Division president and to all members of CNIC.

Document on radical nomenclature (W. Koppenol)

This document had been published as 'IUPAC Recommendations 2000' in *Pure Appl. Chem.* **72** # 3 (2000) 437-446.

Document on muonium nomenclature (W. Koppenol)
The document had been sent to 15 reviewers according to the standard procedures for IUPAC recommendations. All reviewers had answered within the deadline given.

Alan McNaught had proposed to change the word 'muonation' and the prefix 'muono' (both referring to exchange of a hydrogen atom in a molecule for muonium) to 'muoni**i**ation' and 'muoni**i**o', respectively. Reference was made to IUPAC nomenclature of hydrogen isotopes as recommended in

J.F. Burnett, R.A.Y. Jones, *Pure Appl.Chem.* **60** # 7 (1988) 1115-1116.

McNaught's suggestion was agreed to by the Commission after some discussion, during which it was pointed out that 'o' and 'io' forms both have precedence: 'chloro', 'bromo' *etc.*, as used in substitutive nomenclature; 'deutero' as used commonly in organic nomenclature, although possibly not recommended by IUPAC; 'chlorio', 'bromio', 'deuterio' *etc.*, as prescribed in Table VII of the Red Book. (It was left as a task for the group revising the Red Book to consider whether Table VII should be abridged or otherwise revised so as not to make conflicting recommendations.)

The document had been sent to IDCNS and to IUPAP and Koppenol was to further send it to Commission V.7 (Radiochemistry and Nuclear Techniques). Also, it was mentioned that Gerd Rosenblatt is very interested in the subject. Connelly asked whether comments had been received from Gerry Moss, who had expressed interest. [Koppenol has later received these comments from Moss.]

Document on the naming of new elements (W. Koppenol)
Comments had been received from CNIC members and from Jeff Leigh and Gerd Rosenblatt. Further revisions were made during the meeting, partly to ensure that there is language to accomodate the reorganizations taking place within IUPAC. It was also remarked that in cases of shared priority of the discovery of new elements, all discoverers should of course be invited to suggest names.

The document must now be sent to 15 reviewers according to IUPAC procedures. The chairman will approach the Division president and ask for help in assembling the list of reviewers. Several candidates were suggested by CNIC, including Norman Greenwood, Yves Jeannin, A. Vértes, Z. Boksay, Darlean Hoffman, Peter Armbruster, and in general scientists from the labs working with heavy-element synthesis.

After taking comments received from the 15 experts into consideration, Koppenol will send the document on to IDCNS.

Naming of elements # 110, # 111, # 112
An IUPAC/IUPAP joint working party chaired by P.J. Karol has credited *Gesellschaft für Schwerionenforschung* in Darmstadt, Germany (collaboration of S. Hoffman *et al.*) with priority for the discovery of element # 110. Priority for the discovery of # 111 and # 112 has not been established. (A document from the working party dated 5 July 2000 was handed out as supporting material.)

The Division of Inorganic Chemistry is waiting for acceptance by IUPAP of the IUPAC/IUPAP joint working party report. Once this has been confirmed, the CNIC chair will invite the Darmstadt group to propose name(s) for element # 110. The letter of invitation will only be sent, however, when the Koppenol document on the naming of new elements is back from IDCNS review, so that the discoverers may clearly see the rules, in particular the principle of never reusing a name that has already been used for another element.

Once suggestions for names for # 110 have been received by the Chair, CNIC members will be asked to make a vote via E-mail, answering "in favour", "against" or "discussion requested". If agreement can be obtained in this way, it could save much time as opposed to waiting until the Brisbane meeting in 2001 for any further discussions.

Computer-assisted nomenclature activities (A. Dress)
Dress reviewed the IUPAC activities initiated at the March 2000 round table discussion in Washington, a summary of which is available on the IUPAC web site:

http://www.iupac.org/organ/ad_hoc_cmt/nomenclature.html

Most notable was the feasibility study headed by Steve Heller regarding the concept of a unique chemical identifier. A meeting originally planned for early 2000 to get on with CNIC's considerations in the area of computer-assisted nomenclature in collaboration with CNOC representatives had been postponed until June, when it was held in Bielefeld, Germany. Participants included Dress himself and a number of other mathematicians interested in structure classification and encoding, a few local chemists, Heller, T. Damhus, and Janusz Wisniewski from the (then) Beilstein Institute (also representing CNOC). A summary by Damhus had been circulated to a number of people and has later been made available on the IUPAC web site:

http://www.iupac.org/organ/ad_hoc_cmt/nomenclature/Bielefeld2000.pdf

The Heller feasibility study was to be discussed further at a meeting in Cambridge immediately after the Dublin meeting and was to arrive at a first conclusion to be presented to the IUPAC Bureau at its September meeting. Heller's plan is first to address molecular structures with a defined connectivity table, probably modelling primarily smaller organic molecules. Dress suggested that the best way to utilize the expertise present in the network around the Bielefeld group on classification of structures, in particular generalized polyhedral structures, while not interfering with Heller's activities, would be to set up a separate project to deal with chemical indentifiers for cluster structures – with a view to merging it with Heller's project further down the road. During the meeting, Dress consequently wrote up a project proposal along these lines.

(See summary of projects at the end of these minutes.)

Preferred names
At the Washington meeting (see above under 'Computer-assisted nomenclature activities') it was suggested that CNIC should now work seriously at recommending *preferred names* (*P-names* for

short). Jeff Leigh, who participated in that meeting, had also subsequently in a letter to the Division president and the CNIC chair urged CNIC to initiate work on P-names.

The Commission then discussed this subject. There are numerous cases in inorganic chemistry where the decision about which nomenclature system to use will be completely arbitrary. R. Laitinen illustrated this by the example of $SiCl_4$, which can immediately be named according to three different systems (coordination or additive nomenclature; binary or compositional nomenclature; and substitutive nomenclature; see further remarks below on these terms) as

tetrachlorosilicon (in the future probably tetrachloridosilicon)
silicon tetrachloride
tetrachlorosilane

Only personal taste or point of view can decide which alternative to choose, and at least the first two systems are so deeply rooted in inorganic nomenclature that they will certainly both persist. The Commission acknowledged, however, the community's need for P-names, *e.g.* for legal purposes. Consequently, the subject will be addressed, and a project group will be set up to work on it. It was stressed, on the other hand, that it should not be allowed to impact on progress with the Red Book revision, which must have highest priority.

M. Bennett, G. Bergerhoff, J. Wisniewski should be asked to be involved with the P-names.

Suitable test material for discussion of P-names is available in a document authored by Fodor-Csányi listing a number of specific inorganic compounds and IUPAC names for them, and the project group will use this document as a starting point.

See also remarks below regarding organic P-names.

Connelly remarked that with the Red Book revision project already set in a firm time frame, the goal being to have a complete draft of the revised book ready for the Brisbane meting in 2001, there was not time to incorporate P-names in general. The Red Book revision group will, however, to a limited extent take the P-names aspect into consideration, cf. the action list below. Also, for organic compounds named in the Red Book, primarily organic ligands, P-names as prescribed by CNOC will of course be used.

Organic P-names (discussion)
T. Damhus had issued a document listing examples of purely inorganic compounds that had been named in the CNOC P-names document (in the version shared with CNIC after the Berlin meeting in 1999), including a number of parent hydrides and a large number of oxoacids. Obviously, such names need to be considered by CNIC in connection with the CNIC P-names project. J. Wisniewski was present during part of the discussion and clearly indicated to CNIC that the CNOC document was to be finalized at the upcoming CNOC meeting in Frankfurt, so that it would be difficult to ask for revisions of a fundamental nature. However, it had already earlier been stated that CNIC would be given the chance to comment on the document afterwards. Based on these facts, CNIC in the end decided to forward a message to CNOC that we will ask for cross-references to be made in the CNOC document in cases where we can not within a reasonable time frame obtain agreement as to

what the preferred names should be. It should also be made clear to everybody that for the time being, we do not think it is possible to make a coherent system for P-names across inorganic and organic chemistry.

It was anticipated that the CNIC P-names would probably be based in general on additive nomenclature principles, so that *e.g.* tetraboretane would become

1,2,3,4-tetrahydridotetrabory-[04]cycle

and phosphinic acid would become

dihydridohydroxidooxidophosphorus.

Additive nomenclature is well established and documented for coordination compounds, inorganic rings and chains and inorganic radicals.

N. Connelly will check about the use of 'diazane' in Red Book II. The CNOC document has 'hydrazine' as the preferred name. It was also decided to inquire of CNOC why 'indigane' was chosen rather than 'indiane'.

Red Book I revision (N. Connelly* et al.*)

A summary of action steps and an agreed timetable follow this section.

Specific decisions made at the Dublin meeting regarding nomenclature, symbols, terminology, *etc.* in the Red Book revision:

1. Agreement was reached on new proposals for nesting order of enclosing marks, made to simplify conventions and to obtain consistency with the *Blue Guide*:

– in names ( ), [( )], { [( )] }, ({ [( )] }), ...
– in formulae of coordination entities, always [ ] for enclosing the entire coordination entity (and only for that), *i.e.* [ ], [( )], [{ ( ) }], [({ ( ) })], [{ ({ ( ) }) }], ...

In formulae for ions, parentheses are allowed, *e.g.* $(NO_3)^-$.

2. Greek letters will not be italicized.

3. Ligands to be ordered alphabetically in both names and formulae with no distinction between anionic ligands and other ligands (because it is not always obvious what the charge of the ligand is, in particular in organometallic chemistry).
Alphabetization based on actual representation of ligand (so MeCN, CH_3CN, NCMe will be placed differently; use of abbreviations in formulae encouraged, with donor atom preferably placed first).
Terminal ligands retain their position as always closest to metal in names as well as in formulae.

4. The term 'compositional nomenclature' to be used throughout for names of the 'tin tetrachloride' type; the term 'binary' to be omitted except for initial mention in footnote. (In the discussion about this, it was pointed out that the term 'binary' has the virtue of reminding that this nomenclature formally divides constituents into two classes, cationic or electropositive and anionic or electronegative; this connotation is lost with the designation 'compositional').

5. The term 'additive nomenclature' to be used throughout instead of 'coordination nomenclature' after initial mention of the latter in footnote. In the discussion of this, it was pointed out

> (1) that coordination nomenclature is not formally a purely additive nomenclature, because some constituents of the names are modified according to certain rules: ligand names are formed by changing 'ide' to 'ido' and 'ate' to 'ato', and negatively charged coordination entities are given the suffix 'ate';
> (2) if one disregards this point of view, however, there are several systems in use which must be termed 'additive', so that coordination nomenclature is only one of them (another one being the rings-and-chains nomenclature, a third one being conjunctive nomenclature), and a phrase such as 'named by additive nomenclature' could become ambiguous in some cases.

6. Inorganic oxoacids: Damhus presented a document (*Note on nomenclature of inorganic oxoacids*....., dated July 2000) that detailed the various systems for naming inorganic oxoacids presented in the Red Book. These can be exemplified by the following names for the compound $P(OH)_3$:

> phosphorous acid [traditional name, analogous to names like 'ferrous' which have been discouraged by IUPAC for half a century]
>
> trioxophosphoric(3–) acid ['acid nomenclature' name]
>
> trihydroxophosphorus [additive nomenclature]
>
> trihydrogen trioxophosphate(3–) ['hydrogen name' based on additive name for corresponding maximally dehydronized anion]

Following the discussion at the meeting, Damhus will prepare a version of the Red Book chapter on oxoacids in which the 'acid nomenclature' is basically dismissed in a footnote as never used, whereas the other three types will all be presented, but with the additive names tentatively designated as P-names.

7. The term 'seniority' will be done away with, to use only 'priority'.

8. Even though linguistically inconsistent, the term 'bidentate' will be used rather than 'didentate' (the latter was proposed in the current Red Book, but never widely adopted). Initial mention of the latter in footnote.

9. Anion ligand names of the 'chloro' type will be changed throughout to 'chlorido' *etc.*; the former type will still be mentioned as an allowed alternative, awaiting reactions from reviewers (or indeed readers of these minutes) – a global correction back to the 'chloro' form could still easily be made. Reference to be made to the table on p.1565 in Salzer's paper (see above under Minutes 1999), where the 'chlorido' type is given as 'systematic ligand name' and the 'chloro' type as 'alternative ligand name'.

10. The *eta* and *kappa* conventions need clarification. Casey and Kaesz will provide a first written exposition of these conventions and Hartshorn will then work that into Chapter 10.

11. The section on inorganic polymers will be left out of the revised Red Book and left for future publication following collaboration with the Macromolecular Nomenclature Commission.

12. Tables.
Layout of periodic table discussed, details still need to be settled.
Table I: move alternative names azote, theion (which are needed to explain certain parts of nomenclature) to somewhere else.
Table VII is needed, but it must be considered whether all or only some of the 'io' substituent group names presented here should be included (cf. above under muonium document).
Ligand abbreviations (tables I-10.4, I-10.5, X): Fodor-Csányi indicated that these lists were too long. Damhus presented an overview of present rules for naming anions and anionic ligands which will be used in further work with the organic anionic ligands (this overview is included as an Appendix in these minutes).

It should be pointed out to other parties making use of inorganic nomenclature that from now on and until the revised Red Book is a reality, one should not make reference to the Red Book or quote it, but rather seek advice from CNIC regarding specific questions.

Summary of duties agreed on in connection with Red Book revision
– Front pages (preface and introduction). Connelly with help from Kaesz and Koppenol.
Kaesz to draft guide to using the book (flow diagram).
– Tables (periodic table and tables at back of book). Connelly.
N.B. Table 8 to be redrafted by Kaesz and Fodor-Csányi to show use of P-names;
Koppenol to send radical names to Kaesz for incorporation.
– Chapter 1. Connelly – but someone else (**???**) to check/comment on/add to descriptive/introductory part.
– Chapter 2. Connelly.
– Chapter 3. Connelly, but pages 39-41 (allotropes, *etc.*) to be checked by Laitinen.
– Chapter 4. Connelly.
– Chapters 5, 7, 8 and part of Chapter 11 (boron). Laitinen. Radical names from Koppenol.
To include presentation of the various nomenclature systems available for inorganic compounds.
(*N.B.* Rest of old boron chapter to be rewritten in future by **???**, for publication in *PAC* as advanced nomenclature document. Also connection to be made therein to the polyhedral descriptors to be developed in the computer-assisted nomenclature project.)

– Chapter 6. Connelly to recontact Ruediger Kniep to ask for any minor corrections he may have. Chapter 6 to be rewritten by Kniep and others in future, for publication in *PAC* – possible project. Kniep has agreed to participate in that in correspondence with Connelly.
– Chapter 9 (oxoacids). Damhus.
– Chapter 10a (coordination compounds). Hartshorn (with help from Damhus on stereochemistry); *kappa* and *eta* nomenclature to be clarified by Hartshorn with help from Kaesz and Casey. Consider working in flow-diagram approach.
– Chapter 10b (organometallic compounds, probably as a chapter separate from 10a). Connelly and Hutton. To be based on Salzer's published document.
– Abbreviations section. Names of fully hydronated ligands to be deleted from table. Connelly to finalize draft (after Dublin comments). Draft to be checked by Damhus and sent to Casey for queries on organic names.
– Index. Connelly.
– Glossary. Connelly, if glossary needed (tables V and IX to stay).

Timetable for completion
– All drafts to be sent to Connelly by ***January 1, 2001*** for editing.
– Meeting of subgroup to consider Connelly's edited draft (of whole book) in March-April.
– Updated draft (by Connelly, after above meeting) to be issued before Brisbane meeting.

Document on nomenclature of metallacycles of the transition elements
A new version of this document had been prepared in August 2000 by CNIC member Y. Yamamoto, who was not able to attend the meeting. The document was discussed in a smaller group and it was decided that it needs further revision. E. Nordlander will collect comments and produce a new version.

Presentations by J. Wisniewski
[*on Beilstein (now MDL) and Gmelin databases and name-generating software*]

J. Wisniewski (jwisniewski@mdli.com) is a member of CNOC and the author of Beilstein's IUPAC-name-generating software for organic structures, *Autonom*. He explained about the recent acquisition of Beilstein Information by MDL Information Systems, a US-based company which had about 400 employees before the acquisition and thus now has 40 more employees in Frankfurt, Germany.

MDL has recently also bought the right to use the Gmelin database. Under the heading *Focus on inorganic compounds: revival of Gmelin database*, Wisniewski gave the history of the Gmelin Handbook, the Gmelin Institute, and the Gmelin database (in recent years managed by the *Gesellschaft Deutscher Chemiker*). It is the plan to keep the Gmelin database updated henceforth with abstracts from 63 journals, all published by Elsevier (one third in coordination chemistry, one third in inorganic/solid state chemistry, and one third in physical chemistry). Missing data from the years where the database was not being updated are currently being filled in, and completion of this task is planned for 2004. At the present time, the database contains 1.3 million inorganic compounds [the (formerly) Beilstein database contains 10 million organic compounds].

Eventually users will observe no sharp distinction between organic and inorganic nomenclature when entering the MDL databases. Patents will be abstracted to a much larger extent than today. *It is the intention to develop naming software for inorganic compounds to supplement* Autonom. Information on these developments will soon be available at www.mdli.com.

Wisniewski also, in a presentation entitled *Digital naming: IUPAC nomenclature directly from molecular graphs of organic compounds*, explained the principles underlying the construction of the Autonom software and demonstrated its use on a number of examples. At present, the software generates IUPAC-allowed names when given a structure of an organic compound as input, within certain restraints, *e.g.* on total number of atoms and number of rings present in the structure and on the identity of the atoms in the structure. Certain types of symmetrical structure, certain types of ionic structures and other special classes such as radicals cannot be dealt with at the moment, but future versions of the software will eventually solve these problems. Also, it is planned that a 'reverse' Autonom be developed, *i.e.* software that would transform names into structures.

In the ensuing discussion, aspects of the commercial development of nomenclature software vs. IUPAC nomenclature work were touched upon. Should IUPAC promote writing programmes? It adds an extra dimension to nomenclature work if one requires rules to be not only human-friendly, but also computer-friendly.

In all cases, it was agreed that CNIC should keep close contact with Wisniewski on developments of mutual interest.

Other business and agreed actions

– Damhus to send requests to Nordlander for literature searches to assess usage of particular types of names. Nordlander will investigate using the SciFinder software.

– The chairman will write a note regarding the outcome of the CNIC deliberations on P-names at this meeting and circulate it to Casey, Damhus, and Koppenol for comments before sending it to the Division president and to CCINS (the *ad hoc Committee on Chemical Identity and Nomenclature Systems*).

– The Commission asked for clarification regarding the future role of IDCNS (*Interdivisional Committee on Nomenclature and Symbols*) vs. CCINS.

– The Commission inspected the preliminary schedule for the meetings in Brisbane in 2001 issued by John Jost (dated August 9, 2000). CNIC will meet on June 30, July 1, and July 2 and will participate in the open Division meeting in the evening of June 30. Damhus remarked that time must be allocated to joint deliberations with CNOC and may be other commissions. The chairman replied that this must be accommodated within the three days' meetings mentioned above.

- The chairman to communicate to the Division that all CNIC members present at the Dublin meeting were in favour of retaining a status as a permanent body in the Division to ensure continuity in ongoing work and interaction with colleagues working on parallel projects in other divisions. In the discussion of this subject, the chairman mentioned a letter from Jeff Leigh to the Inorganic Division President and to the CNIC chair, dated August 5, 2000, in which concern was also expressed regarding the fate of nomenclature work after the commissions are terminated.

– In any case, CNIC work will continue in four project groups which together include all the members and observers who were present in Dublin. The projects will deal with:

> ***Red Book revision***, already running as a project, headed by N. Connelly.
> ***Computer-aided cluster nomenclature***, project proposal written during the meeting, group to be headed by A. Dress.
> ***Inorganic P-names***, group to be headed (initially) by H. Kaesz.
> ***Organometallic nomenclature***, group to be headed by A. Hutton. Experts on stereochemistry and main-group organometallics still wanted. Maybe A. von Zelewsky could be approached regarding stereochemistry. The eventual outcome of the group's work should be the separate book on organometallic nomenclature which has been planned for about 10 years. The remark was made that making it *The Violet Book* would be unsuitable in view of the present Macromolecular Nomenclature book being *The Purple Book*.

Appendix

Contribution to discussions of naming of oxoacids/oxoanions and of ligands/attached groups in coordination and radical nomenclature at CNIC meeting, Berlin, August 1999; redistributed in shortened version at CNIC meeting, Dublin, August 2000.

1. Existing rules for naming anions, in particular for 'ate' names

2. Existing rules for naming anionic ligands in coordination nomenclature

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1. Existing rules for naming anions

Red Book I-8.3.1: the endings are

'ide' (monoatomic or homopolyatomic species)
- 'ate' (coordination nomenclature, heteropolyatomic species)
- 'ite' (used in some trivial names)

However, *Red Book* I-8.3.3 and *Blue Guide* R-5.8.3 give also the following possibilities (but only these!):

anions formed by loss of hydron(s) from a parent hydride, *e.g.*
methanide, cyclopentadienide, 2,4-dioxopentan-3-ide (!!), stannanide,
diazanide, azanediide

anions formed by the addition of a hydride ion to a parent hydride, *e.g.*
methanuide [= pentahydridocarbonate (1–)]

anions derived from oxoacids by loss of hydron(s), *e.g.*
benzenesulfonate, hydrogencarbonate, acetate, ethanoate, nitrate,
dithionite, hypochlorite

anions derived by loss of hydron(s) from hydroxy characteristic goups or chalcogen analogues, *e.g.*
methanolate, benzen-1,4-bis(thiolate)

a small number of trivial or contracted names, *e.g.*
hydroxide, cyanide, cyanate, amide, imide,
hydrogensulfide(1–), methoxide

Red Book I-10.4.3: all anionic coordination entities take the ending -ate.

Note: not restricted to oxoanions !

(Reference via I-5.3.5 to Table I-9.2 is necessary for obtaining the required modified central atom names, *i.e.* borate, carbonate, zincate, *etc*. The table contains no entries for oxygen and hydrogen; but I-8.3.3.6 gives the name difluorohydrogenate(1–) for $[HF_2]^-$.)

2. Existing rules for naming anionic ligands in coordination nomenclature

Red Book I-10.4.5.1: the names for anionic ligands, whether inorganic or organic, end in -o. In general, if the anion name ends in -ide, -ite, or -ate, the final e is replaced by -o, giving
-ido, -ito, and -ato.

Red Book I-10.4.5.6: Names for ligands derived from neutral organic compounds but the formal loss of hydrons (other than those names in Sections I-10.4.5.1 and I-8.3) are given the ending -ato.

Note: Certain exceptions to the above rules are accepted, as indicated by explicit statement of names as 'Alternative ligand name' in Tables I-10.1 to I-10.5, *e.g.*

chloro, oxo, thio (acetylacetonato), [protoporphyrin IXato(2−)].

However, a number of names are listed as 'systematic' which are not in accord with any rules, *e.g.*

[methanaminato(1−)]
(no rule supports the anion name 'methanaminate', but rules in I-8.3 would give the name 'methylazanide')

2,4-pentanedionato
(no rule supports the anion name '2,4-pentanedionate', but the anion is named as '2,4-dioxopentan-3-ide' in I-8.3, *cf.* item 1 above)