INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Inorganic Chemistry Division
CNIC – Commission on Nomenclature of Inorganic Chemistry (II.2)

Organic and Biomolecular Chemistry Division
CNOC – Commission on Nomenclature of Organic Chemistry (III.1)

Joint Meeting of CNIC and CNOC

July 1st, 2001

Attendance CNIC:
Titular Members: N. Connelly, T. Damhus, R. M. Hartshorn, A. T. Hutton, H. D. Kaesz.
Associate Members: J. Casey.
National Representatives: R. Laitinen, D. Meyerstein.
Observers: L. I. Elding, B. Donovan-Merkert, W. H. Koppenol, V. L. Pecoraro.

Attendance CNOC:
Titular Members: B. J. Bossenbroek, H. A. Favre, B. J. Herold, J. L. Wisniewski, A. Yerin.
Associate Members: L. Goebels, K.-H. Hellwich, V. Kisakürek, J. Nyitrai, H. Smith.
National Representatives: G. Moss.
Emeritus Members: S. Ikegami, W. H. Powell, O. Weissbach.

Minutes:

The meeting was called to order by the Chairman of Commission II.2 (CNIC), H. D. Kaesz, and the Chairman of Commission III.1 (CNOC), H. A. Favre, at the Queensland University of Technology in Brisbane, Australia at 09:00 a. m. on Sunday, July 1st, 2001.

The main subject of the meeting was the CNOC P-Names (preferred names) document and its areas of overlap with currently ongoing work in CNIC regarding the revision of Red Book I.

H. A. Favre explained that the P-Names document was now almost finished in a form ready for review outside CNOC. The document runs to approx. 950 pages (without an index).

T. Damhus, Secretary of CNIC, explained that CNIC had been asked to also consider the generation of P-names for inorganic compounds. G. Moss added that the round table discussion in Washington in March 2000 had revealed a strong desire among nomenclature users for IUPAC to produce just one name for each compound, which had led to the request to CNIC.

P-names are in general only intended for uses where it is compulsory to have a single name for each compound, *e. g*. for legal purposes as in connection with patents, environmental regulation and others. Other names which are considered acceptable may still be used in other contexts.

CNIC, however, regarded it as too ambitious to have P-names in the revised Red Book I, except maybe for restricted classes of compounds. N. Connelly of CNIC, main editor of the revised Red Book I, explained that there is a contract with the Royal Society of Chemistry (the designated publisher) to complete the revision by the end of 2001.

Nevertheless, CNIC had been concerned that a large number of purely inorganic compounds, parents as well as derivatives, are explicitly named in the CNOC document, a number of these according to principles that run against the line of the revised Red Book I and the inorganic P-names in cases where CNIC had already had a vision of the latter. H. A. Favre pointed out that it was often necessary to compare different parts of the CNOC document in order to fully appreciate the background for particular principles or names set forth. T. Damhus told that CNIC had received before the meeting only selected chapters of the CNOC document, and so late that the CNIC members had not yet had a chance to read these carefully.

It was eventually understood that the areas of overlap had to be discussed further by both Commissions. The goal of complete agreement with respect to all contentious issues may not be reached, however, before the documents go to public review. In that case it was considered of utmost importance that the new edition of Red Book I and the P-Names document of CNOC should both contain ample cross-references to the other document, and state explicitly the existing differences between options. For the P-Names document of CNOC this would mean that, if there are acceptable alternatives to a given name, the one according to the revised Red Book I should also be mentioned.

As regards the review of the P-Names document and the revised Red Book I, access to both documents should be granted to both commissions before submission to the Interdivisional Committee on Nomenclature and Symbols (IDCNS) which will still be followed by public review. Submission to IDCNS is expected to be by end of 2001.

A discussion followed of a number of specific inorganic compounds named in the CNOC document, including parent hydrides, and retained names for compounds like hydroxylamine and inorganic oxo-acids. Problems with numbering of atoms in polydentate ligands were also touched upon.

Before going into a more detailed discussion of these problems two specific points were discussed and agreed:

1. It was understood that acronyms and abbreviations used in the revised edition of Red Book I for organic ligands would not need to be changed, even if the acronym or abbreviation were not any more consistent with the P-name (example: maintain ligand abbreviation “thf” even if P-name will be oxolane).
2. It was voted unanimously that there will be only one P-name for each compound.

A suggestion was made by D. Meyerstein (CNIC) to remove all P-names from both the Red Book and the CNOC document and to produce a separate volume on P-names. In a discussion of the purpose of designating P-names several participants pointed out that even though it would often not be the intention that practitioners or educators should use P-names in their daily communication, the mere presence of P-names in IUPAC recommendations would make people consider them as the ones they should use.

After a break a more detailed discussion followed on specific examples:

The first one was about the inorganic parent hydride InH_3:
H. A. Favre presented arguments in favour of the name indigane, instead of indiane or indane, or other possible alternatives:

1. If indiane was used confusion might be caused by "di" being also a multiplicative affix. As a consequence HIn=InH would have to be called diindiene, without being a diene.
2. Indane cannot be used because it is already a widely used name for a certain bicyclic hydrocarbon. Also the 5-membered heterocycle with two double bonds and one indium atom would have to be called indole instead of indigole, indole being already used for another nitrogen heterocycle.
3. Indicane is also a name already used for an existing compound.
4. Indiumane would also not be convenient.

W. H. Koppenol argued against indigane because it would suggest a non-existing relationship to indigo*.

For the preference by CNOC for hydrazine instead of diazane, H. A. Favre presented the following reasons: Wide use of names for many hydrazides RCO-$NHNH_2$, hydrazones RR'C=NNH_2 and for the hydrazino group -$NHNH_2$ and hydrazono group =NNH_2 which should be retained (*e. g.* in $(HO)_3P=NNH_2$ hydrazonophosphoric acid). A name like methyldiazane would, however still be accepted, although the preferred name would be methylhydrazine. Moreover hydrazine is a hazardous compound and for these, as *e. g.* also for acetylene, the traditional names should be retained for safety reasons.

T. Damhus asked about the names which CNOC prefers for the following anions, question which was answered by W. H. Powell:

$H_2N\text{-}NH^-$	hydrazinide
$H_2N\text{-}N^{2-}$	hydrazinediide

H. D. Kaesz suggested the name for the six-membered ring $(SiH_2)_6$ to be discussed. H. A. Favre answered that for rings with up to 10 members the Hantzsch-Widman method would be preferred, according to which the name would be hexasilinane, but that the name cyclohexasilane (used by CAS) would still be considered an acceptable name.

B. J. Herold asked the members of CNIC how they would name noble gas compounds. T. Damhus informed that FArH is known and that one could call it additively fluoridohydridoargon. B. J. Herold proposed that if group 13 to 18 parent hydrides were to be named in a consistent way substitutively, the name would be fluoro-λ^2-argane or fluoro-λ^2-argonane.

Other subjects discussed were the names for H_3SiOH, silanol preferred by CNOC, and $Al(OH)_3$, alumanetriol preferred by CNOC. H. A. Favre explained that by prior mutual agreement, CNOC would use substitutive nomenclature based on parent hydrides of main group elements, except for group 1 and 2. T. Damhus, having participated in and having consulted the minutes of the 1996 CNIC meeting in which H. A. Favre and W. H. Powell also participated, pointed out that the

* Note added after the meeting at the request of G. Moss: Reich and Richter called it indium in 1863 after the indigo-coloured flame test – recognised as different from the colour from caesium.

decision at that time was that organometallic compounds of these main group elements would be named substitutively, not all compounds of these elements.

T. Damhus asked then for the reasons for using the name hydroxylamine instead of azanol for H_2NOH. H. A. Favre replied that, once it had been decided to use the name hydrazine instead of diazane, one would not use the name azane at all, in order to be consistent for nitrogen compounds. For amines the names methanamine, etc. would be used. B. J. Herold pointed out that, since the most abundant elements in bio-organic compounds were C, H, O, N, S and P, there were reasons to treat them in organic nomenclature in a different way from other elements, because of the large and ever growing number of such compounds, which have already been named in a well established systematic way.

T. Damhus asked then which names would be preferred for the following structures. H. A. Favre replied:

H_2NO^-	aminooxidanide
$HONH^-$	hydroxyazanide
NH_2^-	azanide (amide would be kept as a retained, although not preferred name for general use)
CH_3NH^-	methanaminide
CH_3PH^-	methylphosphanide.

In cases where these names appear as ligands in additive nomenclature the ending “e” would be substituted by “o” as in methanaminido.

H. A. Favre coming back to the problem whether to use names for aluminium compounds derived substitutively from alumane, like alumanetriol, instead of a more customary name as aluminium trihydroxide, one would have to draw lines through the periodic table, defining which elements would be considered for nomenclature purposes as metals or non-metals.

The last set of examples discussed was that of inorganic oxoacids CNOC wants to use as functional parents like sulfuric acid, sulfurous acid, as well as phosphoric, phosphorous, phosphonic, phosphonous, phosphinic and phosphinous acids. H. A. Favre, supported by G. Moss, stressed that, given the importance of esters in biochemistry, and the unwillingness of biochemists to change names like adenosine triphosphate and diphosphate, *etc.,* it would be difficult to depart from the existing practice, which involves a very high number of different bio-organic compounds already named systematically and registered with such names in many data-bases.

For polydentate anionic ligands unsolved problems of how to give locants to oxygen atoms were identified as shown by the following examples: In tartaric acid the problem is easy to solve by referring the locants to those of the adjacent atom of the carbon chain, and thus number them as O-1, O-2, O-3, and O-4 (or 1-O, 2-O, 3-O, and 4-O). In the case of triphosphoric acid one will have to decide between two possibilities: either to number the phosphorus atoms from 1 to 3, and therefore give to the oxygen atoms which are not part of the chain the locants O-1, O-2, and O-3 (or 1-O, 2-O, and 3-O), or to number the atoms of the chain from 1 to 5 (including both phosphorus and oxygen atoms) starting with the phosphorus atom at one end and finishing with the one at the other end, and thus have O-1, O-3, and O-5 (or 1-O, 3-O, and 5-O). G. Moss quoted as an example the steroid parent furostan where there is no locant for the oxygen atom between C-21 and C-23. The examples of hydroxymethanetricarboxylic (A. Yerin) and 2-hydroxypropane-1,2,3-tricarboxylic (citric) acid (K.-H. Hellwich) were also quoted.

Both commissions concluded the session by agreeing on the urgent need to continue the discussion of areas of overlap in a more restricted group with representatives from the areas of inorganic and organic chemistry, as well as biochemistry. It was suggested by H.D. Kaesz and H.A. Favre that T. Damhus and R.M. Hartshorn from CNIC, H.A. Favre and W.H. Powell from CNOC, and G. Moss to represent biochemistry, be appointed to the Task Group.*

Submitted on September, 10th, 2001 by

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Ture Damhus, Secretary CNIC

and

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Bernardo J. Herold, Secretary CNOC

Approved on September, , 2001 by

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Herbert D. Kaesz, Chairman CNIC

and

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Henri A. Favre, Chairman CNOC

* Note added after the meeting: T. Damhus suggests for the agenda of this task group discussions of the P-names document and the revised Red Book I, prior to their submission to IDCNS.