

Brief summary of meeting of IUPAC project group, Cambridge, January 27-28, 2002

(Project # 2001-031-1-800: *Alignment of nomenclature in areas of overlap between the preferred names for organic nomenclature and the revision of the nomenclature of inorganic chemistry.*)

Participants

Henri Favre (HF), **Warren H. Powell (WHP)**, **Richard Hartshorn (RH)**, **Ture Damhus (TD; chairman)**, **Gerry P. Moss (GPM)**; **Alan D. McNaught (ADM)**, **Neil G. Connelly (NGC)**, **Herbert D. Kaesz (HDK)** (GPM, NGC, HDK only January 27).

The first five participants on the list constitute the project group with **HF** and **WHP** representing the former Commission on Nomenclature of Organic Chemistry and its project on writing a new Blue Book to replace the Blue Book from 1979 and the Blue Guide from 1993, **GPM** representing the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature, and **RH** and **TD** representing the team working at a revision of the Red Book from 1990 (Red Book I).

NGC is editor-in-chief of the revised Red Book I and **HDK** was chairman of the former Commission on Nomenclature of Inorganic Chemistry (CNIC) where the Red Book I revision project was initiated.

ADM is president of Division VIII on *Chemical nomenclature and structure representation* and also hosted the meeting at the facilities of The Royal Society of Chemistry in Cambridge.

(Chairman's comment: Most attendees considered the meeting to have provided useful discussions and clarification of a number of issues. Attempts were made to compose proper minutes after the meeting, but failed due to disagreement on a number of details in the wording. The present summary is the sole responsibility of the chairman and is mostly kept rather brief.)

1. Review of production plans for the Red and Blue Book

NGC explained that the current timetable for the Red Book I revision called for submission of the manuscript for review in June 2002 and submission to the RSC for publication in December 2002.

RB I is out of print and further delays in the production of the revision should be avoided. As a consequence, the RB I team stood firmly on the decision that ***inorganic preferred names will not be given in the revision***, but must be left for a future project group to deal with.

The Blue Book timetable involves completion of a technically edited draft by April 2002 (could be postponed a couple of months); reviews in by September 2002; final draft December 2002; copyediting completed March 2003; galley proofs corrected September 2003. A publisher has not yet been chosen. Several attendees pointed out that it would be advantageous to have The Royal Society of Chemistry also publish the Blue Book.

The review process was also discussed. One part of the public review could be posting the entire Red and Blue books on the noticeboard of the Division VIII advisory subcommittee for its 40-odd members to review. In addition, **NGC** suggested to consider actually offering individuals a modest compensation, e.g. £ 100, for reviewing one of the books.

When the books are presented for review, a cover letter should clearly state where substantial changes have been made relative to previous recommendations (*e.g.* 'chloro' to 'chlorido' in additive nomenclature). NGC is collecting items for such a cover letter for the Red Book. In some cases, it may still be necessary to just state that "further work on this topic is in progress" (*e.g.* metallacycles, cf. item 4 below).

2. Preferred names and preselected names

The point of this discussion was to ensure that later work on preferred names in inorganic nomenclature (cf. above) was not unduly anticipated in the Blue Book, *i.e.* to ensure that ***no inorganic (non-carbon-containing) compounds were given preferred names*** in the Blue Book.

A device was discussed which would enable the organic rules to institute certain inorganic hydride parent names (such as 'hexasilane') and inorganic oxoacid parent names (such as 'phosphinic acid') as *preselected* for the specific application as parent names for providing preferred names of organic derivatives by substitutive or replacement or functional class nomenclature, without designating them as preferred names for the inorganic compounds themselves at the present time.

It is important to stress that the intention here was just to free the present Red Book I revision team from any considerations about preferred names at this time. It may well be that the parent names now preselected by the Blue Book team, or a number of them, will later be preferred names (for example, 'trisiloxane', 'diphosphoric acid'). Furthermore, the names of parent oxoacids to be used in organic nomenclature will also be mentioned (and indexed) in the revised Red Book I, in some cases in the text and in all cases in the revised and enlarged Table VIII.

Whereas the above *concepts* were applauded as useful and a major step ahead, there were varying opinions on the terms 'preferred' and 'preselected' themselves. It was suggested that the Division (VIII) should take responsibility to eventually consult more widely with the community and ask for better alternatives.

3. Hydrogen names for acids and partially dehydrated acids

Correspondence after the meeting has shown that this long-standing issue is not yet fully resolved. The discussion at the meeting dealt with

- (1) inorganic names with 'hydrogen' joined directly to the name of an anion, *e.g.* 'dihydrogenphosphate' or, fully systematically (in a format currently proposed in the revised Red Book I), 'dihydrogen(tetraoxidophosphate)(1-);
- (2) partially dehydrated organic acids, by present rules named with the word 'hydrogen' separate from the rest of the name, *e.g.* 'hydrogen phthalate';
- (3) partial esters in the names of which 'hydrogen' is also a separate word, *e.g.* 'methyl hydrogen sulfate', 'ethyl hydrogen phthalate';

It may happen that there will continue to be a difference between the naming of inorganic and organic compounds here. It was pointed out that in certain languages (Finnish, Scandinavian languages, German), the chemical names in question are written in one word anyway, so some of

the above problems disappear, but also the possibility of using the space for any kind of distinction is absent.

4. Organometallic nomenclature

Chapter 11 of the revised Red Book I and Sections P-68 and P-69 of the new Blue Book are planned to address the nomenclature of organometallic compounds in the broad sense of the term, *i.e.* compounds with carbon bonded to elements of groups 1,2,12,13,14,15,16, and the transition elements.

A proposal drafted by WHP in November 2001 will provide the basis for selecting preferred names for organometallic compounds. Following the meeting, a revised version of this proposal has been posted on the noticeboard of the Division VIII advisory subcommittee for everybody to consider.

A special subject is *metallacycles*, *i.e.* carbocyclic compounds in which one or more carbon atoms have been replaced by transition metal atoms. A subgroup of the former CNIC had been assigned the task of working out the rules for metallacycle nomenclature (that is, names based on using 'a' replacement terms for the elements substituting carbon), and they had encountered certain problems that would probably only be resolved later when the a project group on organometallic nomenclature started working. That is, the revised Red Book would not give a full treatment of this subject at this time.

5. Red Book chapter on substitutive nomenclature

This chapter, in a draft form, was reviewed on January 28. Numerous specific rules and names were inspected and hopefully brought into correspondence with what will be prescribed in the revised Blue Book. WHP provided a number of references regarding boron nomenclature, including the treatment in Chapter 11 of **P. Block, W.H. Powell, W. C. Fernelius: *Inorganic Chemical Nomenclature – Principles and Practice*** [ACS, Washington, 1990]. If not for the brief treatment foreseen in the revised Red Book I, this input will be of use in the later project of providing a fuller update on advanced nomenclature of boron hydrides and their derivatives.

6. Red Book table of ligand abbreviations and ligand names

This table was likewise examined in the January 28 session and a number of queries dealt with.