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Minutes of meeting of IUPAC project group,

Cambridge, September 29-30, 2001

(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**), **Gerry P. Moss** (**GPM**), **Richard Hartshorn** (**RH**), **Ture Damhus** (**TD**), **Neil G. Connelly** (**NGC**), **Alan D. McNaught** (**ADM**).

The first five participants on the list constitute the project group with **HF**, **WHP**, and **GPM** representing Division III and its project on writing a new Blue Book to replace the Blue Book from 1979 and the Blue Guide from 1993, and **RH** and **TD** representing the team from Division II 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 participated as part of that revision project.
ADM is president of the newly established Division VIII on *Systematic nomenclature and structure representation* under which the present project naturally belongs.

1. Formalities

TD started by thanking **ADM** for providing meeting facilities at the Royal Society of Chemistry's quarters in Cambridge.
Other formalities included questions regarding coverage by IUPAC of the travel and subsistence expenses. The fact that this meeting was adjacent to another IUPAC meeting for some of the persons present, and also that the meeting had had to be planned on short notice because of the urgent nature of the project, had given rise to excessive correspondence and doubt as to how claim forms should be filled out, *etc.* IUPAC may want to consider establishing more flexible ways of handling this kind of situation in the future.

2. The concept of P-names; overlap areas between the Blue and Red Books

A brainstorming session was held with the purpose of generating ideas on how to handle the overlap areas between the new Blue Book and the revised Red Book I. Also, the representatives from the organic side explained thoroughly the concept of ***preferred names*** (henceforth abbreviated ***P-names*** in these minutes). P-names are to be offered to the community for users who require one and only one name for each compound (could be for listing compounds in government regulations of industrial chemicals, pesticides, drugs, *etc.*; for patent purposes; for journal editors; ...).

Often acceptable alternative names will still be presented. However, it is anticipated that many users will look to the P-names and be willing to use them if they are not too cumbersome, so a reasonable compromise between completely systematic names and well-entrenched, but not necessarily systematic names, should be striven for. When traditional names such as methane, acetic acid, acetylene, or phosphoric acid are retained, they will also be the P-names for the compounds in question. The tendency seen throughout the last century towards narrowing the

selection of accepted non-systematic names will be continued when designating P-names in the new Blue Book now under preparation, however. As examples, the book will not have acetone or isopropyl as preferred names, but propane-2-one and propane-2-yl, respectively.

It is worth noting that in the new Blue Book, P-names are only given to compounds defined as specific molecular structures (in some cases up to tautomerism). This will also be important when considering eventually P-names for inorganic compounds, where *e.g.* the formula $AlCl_3$ could cover both a compound defined only by being composed of aluminium and chlorine in the molar ratio 1:3; the specific molecule $AlCl_3$, if one wanted to discuss that; or the molecule Al_2Cl_6. Names designating these different interpretations of the formula could be aluminium trichloride, trichloridoaluminium, and di-μ-chloridobis(dichloridoaluminium). It would not be possible to operate with only one P-name corresponding to the formula $AlCl_3$.

The discussion then evolved into more specific consideration of classes of compounds where an effort must be made to make the two different naming approaches taken in the Blue and Red books meet.

For example, according to the system presented in the new Blue Book, H_3PO_4 is phosphoric acid, and derivatives thereof may be named by replacement infixes, *e.g.* phosphorofluoridic acid for H_2PFO_3, which again naturally would lead to the name phosphorofluoridate for $[PFO_3]^{2-}$ (the 'monofluorophosphate' of everyday toothpaste advertisements). The latter compound, however, would be named additively in the Red Book, *i.e.* as fluoridotrioxidophosphate(2−).

Full replacement of the coordination sphere by fluoride leads to $[PF_6]^-$, which additively would be named analogously, *i.e.* as hexafluoridophosphate(1−). By Blue Book rules, one would shift over to substitutive nomenclature based on the parent hydride PH_5, leading to the name hexafluoro-λ^6-phosphanuide.

The ion $[PS_4]^-$ could be named phosphorotetrathioate or tetrasulfidophosphate(3−), but the first name would not highlight the analogy with $[VS_4]^-$, which certainly would be named tetrasulfidovanadate(3−).

The compounds $[BH_4]^-$ and $[BPh_4]^-$ would be named as boranuide and tetraphenylboranuide by Blue Book rules, but are traditionally named additively in inorganic nomenclature and would thus in the Red Book be named tetrahydridoborate(1−) and tetraphenylborate(1−), respectively.

TD handed out excerpts of a chapter on inorganic oxoacids for the Red Book I revision in which the parent acids as well as derivatives thereof were named additively. The background for this was that CNIC (the Commission on Nomenclature of Inorganic Chemistry) had been in favor of presenting a unified approach to the systematic naming of inorganic acids and their derivatives, as opposed to the confusing multitude of names given in the present Red Book I. Thus, the CNIC approach had, in fact, been a move away from the old names that the Blue Book team was suggesting to retain (phosphinic acid, sulfurous acid, *etc.*), and away from the replacement and functional class nomenclatures for derivatives (leading to names such as phosphinodithioic acid, imidosulfurous fluoride isocyanate, *etc.*). In particular, the endings 'ic' and 'ous' were seen as analogous to the 'ic' and 'ous' endings for metal ion names (cupric/cuprous *etc.*), which were discouraged already in the 1970 Red Book. In the cases of phosphorous and telluric acids, the names are even ambiguous (both have been used for more than one compound).

The rest of the discussion is summarized in connection with the listing of the agreed action steps below (item 4).

3. Discussion of names of organic ligands

The table for Red Book I containing a list of ligand names, abbreviations for these to be used in formulae of coordination compounds containing the ligands, and associated drawings of the structures was inspected. A number of names of organic ligands were corrected according to the rules of the new Blue Book.

4. Action steps agreed upon

4.1 Parent hydrides

WHP/HF will consider rules for naming of $[AB]_nA$-type heterogeneous parent hydrides and return very soon with a proposal for a rule telling exactly for which compounds these names are allowed and for which they are preferred. The Red Book I team needs this input for their presentation of parent hydrides in the chapter on substitutive nomenclature.

4.2 Inorganic oxoacids and derivatives

WHP/HF will formulate new rules to exclude the 'ous' acid names in groups 15 and 16 and will consider the implications of doing so in group 17 as well. Also, the name orthosilicic acid should be left out. Preferred names for derivatives of the acids left out with a carbon bonded to the central atom in question will be substitutive on the basis of the relevant parent hydride (phosphane, λ^4-tellane, *etc.*). Preferred names for the left-out acids themselves and other derivatives of these will not be prescribed at this time.

The remaining acids (phosphoric, diphosphoric, triphosphoric, sulfuric, *etc.*) will retain their 'ic' names, which will therefore be preferred names, and preferred names for derivatives with a carbon atom bonded to the central atom in question will be constructed on the basis of these names for the parent acids. Other derivatives will not be given P-names at this time.

The name telluric acid will be understood to denote H_2TeO_4, while $[Te(OH)_6]$ will be named differently , either as hexahydroxidotellurium or as hexahydroxy-λ^6-tellane (a P-name will not be given at this time, cf. below).

All replacements in the parent acids with retained names are to be designated by *infixes* in the preferred names (phosphoramidic acid, sulfurothioic acid). Exceptions are the polynuclear acids (*e.g.* diphosphoric acid) and possibly nitric acid and cyanic acid.

The revised rules should be drafted and circulated for commenting by the entire group by November 1, 2001. The Red Book I team needs these rules for revision of their chapter on inorganic acids.

4.3 Compounds of elements of groups 13-17

It was decided to *not* give P-names at this time for any compounds containing the elements

Al, Ga, In, Tl
Sn, Pb
Sb, Bi

Te, Po
At

except for their binary hydrides. Section P-68 of the new Blue Book should instead illustrate how both substitutive and additive nomenclature can be used to name compounds in this "grey zone". **TD** will go through section P-68 and provide, on behalf of the Red Book I team, all the additive names that should be given as alternatives to the substitutive ones already there. The additions will be made electronically and the resulting document sent to everybody in the group for consideration before November 1.

4.4 Organometallic compounds

The present chapter 11 of the new Blue Book will be looked at by the Red Book I team including **Alan Hutton**. The naming of all the compound types in chapter 11 will be covered in the revised Red Book, so the chapter is not necessary from that point of view. However, the Red Book group will return with a proposal on how to cast the chapter in order for it to fulfill the organic team's original intention that it should show the differences in naming across the various classes of compounds, using both substitutive and additive nomenclature.

(Compounds of elements of group 1 and 2 and of the transition elements will probably be treated in the organometallics chapter in the revised Red Book I. Compounds of other main group elements will be exemplified in the chapters on substitutive and additive nomenclature. The Red Book I group should take care to include polynuclear compounds which contain central atoms from different groups in the periodic table, *e.g.* Sn and Bi, Ga and Hg, *etc.*)

4.5 Stereochemistry

After a general discussion on *e.g.* definition of *TBPY* vs. *SPY* and on T-shaped and seesaw-shaped molecules, three distinct upcoming activities were outlined.

- Stereochemistry is treated in the revised Red Book I in the chapter on coordination compounds, although some of the descriptors presented could well find use outside this class of compounds (if taken in the narrowest sense of the term). It was nevertheless decided to leave the stereochemistry section in that chapter. **NGC** and **RH** will tidy up the section and eventually send it to **GPM**. Introduction of polyhedral symbols for T-shaped molecules and seesaw structures will be worded by **RH** and passed to **GPM** before end of October.
- Stereochemistry, essentially the CIP system, is treated in section P-8 of the new Blue Book. This chapter will be finalized and sent to everyone as soon as possible (**HF**/**GPM**).
- **GPM** is working on a broader stereochemistry document which will be or include a revision of the entire section E of the 1979 Blue Book (aiming for an article in *Pure and Applied Chemistry* or a book). Stereochemistry of coordination and organometallic compounds could be worked into this document.

5. Other subjects of relevance to the updating of the Red and Blue Books

- It was suggested to *generally* remove non-carbon-containing examples from the Blue Book text (except for parent compunds), *e.g.* examples such as

  1,3,4,5,6,7-hexathia-2-selena-8-tellurocan (which by additive nomenclature would be named 1,3,4,5,6,7-hexasulfy-2-seleny-8-telly-[8]cycle)
  $H_2P(S)SH$
  $(H_2NNH)PBr_2$

H_2AsTeH
HSBr
$SO_2(NH_2)_2$
H_4Bi^+

- It was noted that the Red Book will not employ the term ***seniority***, but only the term ***priority***. The Blue Book team pointed out that ***priority*** there will specifically denote priority as defined in the CIP rules, whereas ***seniority*** will be used in connection with the hierarchial ordering of parent hydrides and characteristic groups in the naming process.

- The Blue Book team told that the preferred names for H_3O^+, H_3S^+, ..., NH_4^+, PH_4^+, *etc.*, will be oxidanium, sulfanium, ..., azanium, phosphanium, *etc.*

- **ADM** informed that the RSC has a large database of referees for their scientific journals, and that this could be used to indentify individuals working in particular fields (*e.g.* tellurium compounds); such individuals might be approached to get an early opinion on the proposals for some of the overlap areas considered here.

- It was agreed that there should at the end be a joint preface to both books. **ADM** volunteered to draft this preface when the time comes to write it.