Minutes of the IUPAC Chemical Nomenclature and Structure Representation Division (VIII) Committee Meeting

Budapest, Hungary, August 30-31, 2004

Members Present: Dr Jonathan Brecher, Prof Richard Cammack, Dr Ture Damhus, Prof Richard Hartshorn, Dr Stephen Heller, Prof Herbert Kaesz, Prof Jaroslav Kahovec, Prof Dr Alexander Lawson**,** Dr Alan McNaught (President), Dr Gerard Moss, Prof József Nyitrai, Dr Warren Powell (Secretary), Dr Matthew Toussant, Prof Andrey Yerin

Representatives from other IUPAC bodies present: Prof Bryan Henry (IUPAC Vice President)

National Representatives Present: Prof Len Lindoy, (Australia), Prof Rita H. de Rossi (Argentina)

Invited guests: Dr Jeffrey Wilson (CAS), Dr Kevin Thurlow (Laboratory of the Government Chemist, UK)

Members Absent: Dr Michael Hess, Prof G Jeffrey Leigh, Dr Antony Williams

The fourth meeting of the Division Committee of the IUPAC Division of Chemical Nomenclature and Structure Representation held at the Budapest University of Technology and Economics was convened by President McNaught at 9:00 a.m. on Monday, August 30, 2004.

1.0 President McNaught welcomed the members to this meeting and offered a special welcome to the new members elected for 2004; to Prof Richard Cammack, Chairman of JCBN, a new ex officio member; and to the National Representatives, Prof Len Lindoy (Australia, University of Sidney) and Prof Rita H de Rossi (Argentina, University of Córdoba)

He also noted that Dr Michael Hess, Prof G Jeffrey Leigh, and Dr Antony Williams would be unable to be with us. The attendees introduced themselves and provided a little background information. Housekeeping details regarding breaks and lunch were announced.

2.0 The agenda as circulated was approved with the addition of a report on CAS index nomenclature by Dr. Jeffrey Wilson at item 10.

3.0 The minutes of the Division Committee Meeting in Ottawa, Canada on August 9-10, 2003 as posted at:

http://www.rsc.org/IUPAC8/attachments/DivisionCommitteeMinutesOttawaFinal.rtf
http://www.rsc.org/IUPAC8/attachments/DivisionCommitteeMinutesBostonFinal.pdf

were approved with the following corrections.

(1) Minute 11.0(1). The use of 'preselected' was felt to be unclear. The minute was revised as follows to clarify its meaning:

11.0 (1) Preferred names for inorganic, i.e. noncarbon containing, compounds are not assigned in the preferred names book. Inorganic parent compounds containing hydrogen that may be substituted by organic residues

are termed ‘preselected’; preferred names are given for organic derivatives of such inorganic compounds.

(2) Minute 11.0 (2) Organometallic compounds: The last sentence was to be deleted.

4.0. Matters arising from the Ottawa minutes.

(1) The earlier paper on cluster nomenclature by T. Sloan, W. Powell, and D. Coucovanis was found in the files at CAS and was sent to G. J. Leigh. [see item (3) under Ottawa minute 11.0]. No confirmatory response has been received.

(2) Increased membership of the Division electorate is to be discussed further by the Division Presidents (see Ottawa Minute 4.1).

5.0 IUPAC-IUBMB. The minutes of the meeting of the IUPAC/IUBMB Joint Commission on Biochemical Nomenclature (JCBN) in London, May 1-2, 2004 may be found at:

http://www.rsc.org/IUPAC8/attachments/JCBNMinutesLondon2004(draft).pdf

(1) Dr Richard Cammack offered the following comments.

(a) JCBN is looking for new members, particularly from the biochemical community.

(b) The rules of enzyme nomenclature are being clarified so that new enzymes can be named by the enzyme chemist.

(2) Dr Steve Heller described progress with the new PubChem database of the US National Center for Biotechnology Information

(http://pubchem.ncbi.nlm.nih.gov), managed by Dr Steve Bryant.

(3) The launch of the European Bioinformatics Institute’s ChEBI database (Chemical Entities of Biological Interest) at

http://www.ebi.ac.uk/chebi

was noted. The database will include Preferred IUPAC Names.

(4) Prostaglandins. The document on prostaglandin nomenclature written some years ago by Kurt Loening and Joy Merritt should be reviewed as a potential publication. Even though nomenclature for prostaglandins is handled by general natural product nomenclature (Section F of the 1979 edition as revised), it contained much information on earlier nomenclature for prostaglandins.

6.0 Revised Section F: Natural Products and Related Compounds (IUPAC Recommendations 1999), published in *Pure Appl. Chem.* **71**, 587-643, 1999; web publication:

http://www.chem.qmul.ac.uk/iupac/sectionF.html.

During translation of these recommendations into German, a number of errors and minor problems were discovered by K-H. Hellwich. As a result, a section of “Corrections and Modifications (2002)” was added to the web version of this publication:

http://www.chem.qmul.ac.uk/iupac/sectionF/Ferror.html

and published in *Pure Appl. Chem.* 2004, **76**, 1283.

7.0 Division VIII Projects

7.1 IUPAC-NIST Chemical Identifier. Status report by S. Heller.

A new test version of the IUPAC-NIST Chemical Identifier (INChI, formerly IChI) was made available in July. It replaces the previous test version issued last November. All features planned for inclusion in the final release have now been implemented and the final format for the Identifier has been agreed (it is simply a text string). Also, the Identifier is now called INChI (formerly IChI) to acknowledge the development work at NIST. The test program accepts input in the form of MOLFiles (or SDfiles) and CML files. An Application Program Interface (API) for communicating with external programs is under development (see later).

A single INChI is generated for a single input structure, which can contain multiple components. Identifiers can be created for organic compounds with *Z/E* and sp^3 stereochemistry, tautomers, and isotopes as well as salts, organometallic compounds and protonated forms of a compound.

Test programs (for Microsoft Windows), documentation and sample structure files are available for download at:

http://chemdata.nist.gov/IChI/INChIv11b.zip

Application Program Interface (API). For those interested in generating INChI from their own programs and structure collections, we are developing an API to be issued as a dynamic link library (DLL) and a directly linkable library. Those interested in this software should let the project team (Steve Stein, Dmitrii Tchekhovskoi, Steve Heller, Alan McNaught) know. It would also be helpful to know of operating system and software system requirements. INChI algorithms are implemented in ANSI C.

Comments concerning the INChI are encouraged and the project team will be glad to assist in its testing or implementation.

Other comments arising in the discussion.

(1) ACD (Advanced Chemistry Development) has implemented INChI generation and is advertising its use.

(2) The question of licensing at no cost but with ownership still remaining with IUPAC is being discussed with the IUPAC Secretariat.

(3) It is necessary to recognize that future versions will be needed which should be backwards-compatible.

(4) INChI is very dependent on the structure that is input; it's development should be interlinked with the structure drawing project.

(5) The algorithm doesn't yet handle polymers

(6) The question of other formats for the API is under consideration.

7.2 Preferred IUPAC names for organic compounds. W. H. Powell reported that the new Blue Book was posted on the Division Webboard for review by the Division VIII Committee members and the Division VIII Advisory Subcommittee in June and July, 2003. Comments on Chapters 1-5 were reviewed at a Project Group meeting in Ottawa, August 6-7, 2003. Comments on Chapter 6 and other comments on Chapters 1-5 were reviewed at a meeting of the Project Group in Gaithersburg, MD, November, 2004.

A revised draft is nearing completion; it should be ready to be posted on the IUPAC Web site for public review in the next month or so.

It was suggested that a list of all of the important changes from the 1979 Blue Book and/or the 1993 Guide along with explanations, where needed, be published along with the revised draft.

7.3 Revised Red Book. Ture Damhus reported that the public review for the revised Red Book is over and the comments are being evaluated by the Project Group here in Budapest. He also brought up questions regarding consistency between the New Red Book and the New Blue Book.

(1) Enclosing marks. Ture Damhus offered the following examples from the 1990 red Book, the 1979 Blue Book, and the 1993 Guide.

Red Book 1990, I-2.2.1
Formulae: [{{[( )]}}]; seems to mean [{...{{[( )]}}...}]
Names: {{{[( )]}}}

Blue Guide 1993, R-0.1.5.3
No distinction made between formulae and names; nesting order is [({[( )]})]}, etc.

Comment: R-0.1.5.3 is a subrule under R-0.1.5 which clearly deals with names; formulas are not mentioned. R-0.1.5.2(e) deals with use of brackets to indicate repetition of groups in chains. Although not mentioned in the 1993 Guide, in formulas, groups attached to chain atoms are enclosed in parentheses (see P-16.4.1.8).

Revised Red Book 2004, IR-2.2.1
Formulae: [{({( )})}]
Names: as Blue Guide above

Comment: The real problem in the nesting order {[({[( )]})]} in names is the question of what to do when consecutive enclosing marks of the same kind occur in the name. An example of this concern is the INN moexipril, which, according to the nesting rules, should have the name:

(3S)-2-((2S)-2-{[(1S)-1-(ethoxycarbonyl)-3-phenylpropyl]amino}propanoyl)-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid

but this name involves consecutive parentheses, since outside the {} the next should be () again. The second (2S) should force a jump to []. By using three types of brackets there is always one type left whatever the two outside ones are. Here there is (.....} hence the next is []. Hence, the name probably should be:

(3S)-2-[(2S)-2-{[(1S)-1-(ethoxycarbonyl)-3-phenylpropyl]amino}propanoyl]-6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline-3-carboxylic acid

(2) The multiplicative prefixes 'di, tri, ...' vs. 'bis, tris, ...'

(a) Blue Guide R-0.1.5.1: use parentheses after 'bis, tris, etc.'

Example for discussion:

2,2'-cyclohexane-1,3-diyldiethan-1-ol or
2,2'-cyclohexane-1,3-diyldi(ethan-1-ol) or
2,2'-cyclohexane-1,3-diylbis(ethan-1-ol) or even
2,2'-(cyclohexane-1,3-diyl)bis(ethan-1-ol)

Comment: According to R-0.1.4.1, the first above is correct.

(b) Use 'bis, tris,...' when ambiguity could arise

Examples for discussion:
tetrasulfatocerate(4-) vs. tetrakis(sulfato)cerate(4-)

Covered by R-0.1.4.2. Since tetrasulfato is a ligand from tetrasulfuric acid, four sulfato ligands must be described by tetrakis(sulfato)

thallium tris(iodide)

Comment: (should be thallium tris(iodide) to be compared with thallium (triiodide) [Applies also to the next two examples]

thallium tris(bromide)
thallium tris(chloride)

phosphorus triiodide

(2) Dioxidanium(1+) is neither an additive nor substitutive name; it is a combination of both. The substitutive name would be just dioxidanium.

(3) The term hydrate, and the use of 'hydrate', in systematic names *vs*. the format with a long dash and the name 'water'. (Note that the Gold Book lists neither 'hydrate' nor 'solvate').

The names deuterate and tritiate should not be used. The names (^{2}H)water and (^{3}H)water should be used instead.

(4) The element names sodium/natrium, potassium/kalium, tungsten/wolfram and in particular derived forms such as sodate, potasside, tungsty have been mentioned elsewhere.

There was no discussion on this point.

7.4 Fullerene nomenclature, Part II (W. H. Powell). The public review stage for the paper "Numbering of Fullerenes (Recommendations 2004)" was over on August 31. The Project Group will meet here in Budapest to consider all of the comments received. It should be submitted for publication by the end of September.

7.5 Rotaxanes (2002-007-1-800-C). A. Yerin reported that a draft document entitled "Nomenclature for Rotaxanes (IUPAC Recommendations)" was posted on the Division VIII Webboard in April, 2004. This draft and comments received on it will be discussed at a meeting of the Project Group, September 1, 2004 here in Budapest.

7.6 Stereodescriptors for coordination numbers 7-12 (R. Hartshorn). The project established to review and extend existing recommendations for stereodescriptors for coordination numbers 7-9 and develop recommendations for stereodescriptors for coordination numbers 10-12 has been split up. R. Hartshorn will handle coordination numbers 9-10; G. J. Leigh will deal with coordination numbers 11-12; and René Sommer and Eva Hey-Hawkins will do coordination numbers 7-8. Reports are to be sent to G. J. Leigh by the end of September and a meeting of the Project Group is planned for spring of 2005.

7.7 Macromolecular Projects with Division IV. M. Hess sent a report on discussions of projects from the meeting of the Subcommittee for Macromolecular Terminology held June 28-July 1, 2004 in Bordeaux, France.

7.7.1 Macromolecular rotaxanes, i.e., rotaxanes with repeating unit components (2002-037-1-800)(cf. Rotaxane project above). This project has been put on hold until the project on rotaxanes without repeating unit components is well along. A. Yerin was asked to lead the project when it is revived and G. Moss will also be a member of the project group.

7.7.2 Terminology and Structure-based Nomenclature of Dendritic and Hyperbranched Polymers (2001-081-1-800)(J. Kahovec). This project is almost ready for expert review. It includes structures with and without repeating unit components.

7.7.3 Structure-based Nomenclature for Cyclic Macromolecules (2202-015-1-800)(Werner Mormann). A draft for review by Division VIII

Committee members and the Division VIII Advisory Subcommittee was posted on the Webboard in July, 2003. These recommendations were reviewed by the Division IV Subcommittee on Macromolecular Terminology at its meeting June 28 – July 1 in Bordeaux, France and should be ready for expert review by October 2004. The title for this project seems misleading in that it implies that it deals with large rings, when in reality it deals with large rings containing repeating unit components.

7.7.4 Source-based Nomenclature for Modified Polymer Molecules (1999-05-1-800). This project is better left with the Division IV Subcommittee on Macromolecular Terminology. The new project leader, Prof T. Kitayama, who took over this project following the resignation of T. Wilks at the Ottawa meeting, presented a new, more practical and user-friendly approach to the subject. Hence, the project was restarted on the basis of the new draft; the project will need a project extension. A revised draft will be available for the 2005 meeting of the Subcommittee in Beijing.

7.7.5 Source-based Nomenclature of Single-Strand Organic Polymers (2003-042-1-800) (T. Kitayama). This project originates from a revision of "Source-based Nomenclature for Copolymers", *Pure Appl. Chem.* **1985**, *57*, 1427-1440. The whole concept of the project has been changed, including its title, which will now be Source-based Nomenclature of Organic Homopolymers and Copolymers.

7.8 Cyclic Peptides (2004-024-1-800) (G. P. Moss). This document arises from work carried out under the auspices of the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature. A revised document is now ready for public and ICTNS review.

7.9 Graphic Representation Standards for Chemical Structure Diagrams. (2003-045-3-800). This project started two years ago as a scoping exercise directed by J. Brecher. Following official project approval in March, 2004, work has continued at a slow but steady pace. Recent discussions have focused on areas of stereochemical representation that were not resolved prior to project approval. Representation of non-T4 configurations (octahedral, etc.) received the most attention, followed by issues relating to the display of relative stereochemistry, along with many other areas. The current working draft recommendations continue to be available at:

http://www.angelfire.com/sc3/iupacstructures/

with the stereochemical recommendations starting with:

http://www.angelfire.com/sc3/iupacstructures/stereo/

As of the middle of August, 2004, the stereochemistry recommendations are thought to be close to complete and will be the main focus of a meeting of the Project Group on September 1, 1004 in Budapest. It seems likely that a completed draft of stereochemistry recommendations will be ready to submit for review this year, in accordance with the original project timetable. The proposed recommendations will

likely supersede the existing recommendations given in the "Basic Terminology of Stereochemistry (IUPAC Recommendations 1996)", *Pure Appl. Chem.* **1996**, *68*(12), 2193-2222

(http://www.chem.qmul.ac.uk/iupac/stereo/intro.html)

7.10 Classification, terminology, and nomenclature of borophosphates (2003-034-1-200)

This project will reside in Division II but Division VIII will supply some monetary support and provide a watchful eye for nomenclature issues. At the present time, the main problem is that the proposed Project Leader is ill; a new Project Leader may be needed.

7.11 Comparison procedures for naming hydro derivatives of fused ring systems. A document entitled "A Comparison of Nondetachable Hydro Prefixes (IUPAC), Added Hydrogen (CAS), and Indicated Hydrogen (Beilstein), in Expressing Substitutive Suffixes" prepared several years ago as a publication by the IUPAC Commission on Nomenclature of Organic Chemistry is now planned as a technical report. The introduction needs to be revised and then it should be sent for review of the respective CAS and Beilstein procedures by Karl-Heinz Hellwich and Sandy Lawson for Beilstein and to Jeffrey Wilson for CAS. Although not yet public, the URL for this document is: http://www.chem.qmul.ac.uk./iupac/misc/hydro.html

8.0 Correspondence with the International Mineralogical Association (IMA) Commission on New Materials and Mineral Names. Correspondence between H. Kaesz and Dr. Peter Bayliss relative to the nomenclature proposal "Chemical Adjectival Modifiers on Mineral Species" (see Minute 9.1 of the Boston meeting, 2002) has developed into a proposed paper "Mineral species nomenclature: chemical-element modifiers". It is attached as Appendix I. Comments should be directed to H. Kaesz.

9.0 Future division projects.

9.1 Preferred names for inorganic compounds (T. Damhus). A meeting of those interested in such a project and with varied backgrounds recruited by T. Damhus was held on Sunday, August 29 here in Budapest to prepare a project for the generation of preferred IUPAC names for inorganic compounds. T. Damhus will attempt to write such a project proposal; interested persons are needed to assist and review. It will consist of a core group and a layer or corresponding members. The implementation of REACH, the European Union's proposed new scheme for registration of chemicals, will require a new database providing an opportunity to promote PINs.

9.2 Metallacycles. A project based on the pertinent sections of the paper by A. Salzer will be established led by H. Kaesz and W. Powell. H. Kaesz will draft the project proposal. A previous draft by Yamamoto, McCleverty, et. al., should be sent to H. Kaesz and W. Powell. A draft on metallacyles for CNOC was prepared several years ago by W. Powell. He will try to locate a copy. It was suggested that 'ocenes' not be included in the proposed project, but be a separate project.

9.3 Preferred IUPAC names for polymers. The second edition of the Compendium of Macromolecular Nomenclature (Purple Book) will be published soon. It will not

contain new material, only already published material will be included. J. Kahovec will check to see if the new document on single-strand organic polymers might include preferred IUPAC name designations. There will be a need for review of all macromolecular nomenclature for consistency with the new Blue Book.

9.4 Stereochemistry. The scoping exercise on stereochemistry has been completed and a core group of R. Hartshorn, G. P. Moss, and K-H. Hellwich met in Ottawa on August 8 to plan for future projects. It was determined that the subject was too large to include in one project. Nothing more is expected until the projects on coordination numbers 7-12 and stereochemical representation are further along.

9.5 Revision of carbohydrate nomenclature. Derek Horton wants to do this work. A main question at this time is whether to deal with such a revision as an Appendix to the current recommendations or as a new project. No funding is required and thus no support from Division VIII would be required. However, a time frame for such a work would be needed. Prof Cammack agreed to prepare a project proposal.

9.6 Biochemical compounds glossary. Various activities are in progress related to the creation of glossaries for compounds important to biochemists A request has been made to Chemical Abstracts Service for cooperation with current work at the University of Missouri.

9.7 Inorganic nanomaterials. A proposal for a two-day workshop on nanomaterial nomenclature has been made by the Center for Biological and Environmental Nanotechnology (CBEN), for which see:

http://.rsc.org/IUPAC8/attachemnts/Nanomaterials.pdf

[The minutes of the meeting of the ACS Committee on Nomenclature, Symbols, and Terminology in Philadelphia, August 21, 2004 noted that the meeting originally scheduled in Anaheim would be held on September 29-30 at NIST. Dr. J. Wilson of CAS was to attend this meeting]

It remains an open question as to whether Division VIII should be involved in the nomenclature of nanomaterials. Liaison with the ACS Committee should be useful here.

9.8 Boron Nomenclature. A project proposal and participants are needed.

9.9 Other Projects.

9.9.1 Generalized cluster nomenclature. A copy of a paper by T. Sloan, W. Powell, and D. Coucovanis was sent to G. J. Leigh for use in development of projects in this area

10.0 Developments in Computerized Naming

10.1 Advanced Chemistry Development (ACD). Andrey Yerin described the development of computerized nomenclature at ACD. The work started some 9 years ago concentrating on translating a structure to name. The bases for names are the 1979 recommendations and the 1993 Guide. As the IUPAC Recommendations were published components have been added, for example, replacement nomenclature, phane nomenclature, fullerenes, bridged fused ring

systems, von Baeyer ring systems, spiro ring systems, natural products. Replacement nomenclature is difficult to encode and there are difficulties with skeletal modifications of natural product structures, such as nor, homo, and especially seco. Translation of inorganic and coordination structures is just beginning. As yet, no work on polymer names is being done.

There has not been the degree of response that ACD expected from Tony Williams' offer of the ACD programs to Division VIII Committee members. Some just haven't used them. Some claimed that they did not receive the programs; this might be a problem with downloading. A. McNaught will talk to Tony about continuing his offer. The ACD programs are not available on Mac systems.

ACD provides links to the specific IUPAC rules used to derive specific names. It would be very useful to get figures on the use of the IUPAC rules from ACD.

10.2 AUTONOM was the first to tackle computer generation of names from structure input and relies on identification of functional groups and rings rather than text nomenclature. The names generated are based on Beilstein's interpretation of the IUPAC Recommendations.

10.3 CambridgeSoft. Jonathan Brecher described the status of computerized nomenclature development at Cambridge. CambridgeSoft translates names to structure and does not begin with a specific set of rules. For a batch of names that can be given structures, the success rate is 70% - 90% with an accuracy of 99%. The reverse process, i.e., structure to name, was started only a couple of years ago.

10.4 Chemical Abstracts Services (CAS). Dr. Jeffrey Wilson described the use of the computer for nomenclature purposes at CAS.

10.5 Laboratory of the Government Chemist (LGC). Dr. K. Thurlow described his work in nomenclature for the LGC.

10.6 Openeye Scientific Software. (OGHAM). According to the Web site for OGHAM, which is

http://eyesopen.com/products/applications/oghan.html

the primary features are:

(1) Generation of structure diagrams (2D coordinated) suitable for rendering, from names, connection tables (e.g., SMILES) of 3D structures.

(2) Renders images (GIF), BMP), or (EPS) from either generated or user supplied structure diagrams (2D coordinates)

(3) Gives reasonable names (either traditional or IUPAC) to chemical structures or connection tables.

(4) generates connection tables for named compounds (traditional or IUPAC)

11.0 Publicity. The purpose of publicity is to promote what IUPAC is and does and to promote what Division VIII is and does. The several ideas suggested at the Division Committee's Open Meeting in Ottawa, August, 2004 to accomplish these goals were re-emphasized. Additional suggestions included:

(1) press releases in Chem. Eng. News, Chemistry World, Nature, and Science to coincide with the publication of the revised Red Book and the revised Blue Book

(2) There was no interest from publishers in the suggestion made last year to put a stamp of approval about IUPAC nomenclature on papers or books, etc.

(3) Note differences between CAS index nomenclature and IUPAC nomenclature. An internal report prepared by W. Powell exists at CAS. J. Wilson will look for it.

(4) Lectures on nomenclature, for example, W. Powell gave three lectures in Taiwan in 1995.

(5) Workshops with and presentations to regulatory agencies about IUPAC nomenclature, e.g., A. McNaught's proposed presentation on IUPAC nomenclature to European Customs Chemists.

(6) Develop lists of contacts, for example, with the Chemical Manufacturer's Association.

(7) Send representatives to universities

(8) Put up slides between talks at meetings. Collect examples to present. This could be a Project.

(9) Establish contacts with high school chemistry teacher's associations. The ACS Committee on Nomenclature has had a representative from such associations in New York and Illinois in attendance at their annual meetings.

H. Kaesz agreed to put together a publicity plan to be followed when the new Red and Blue Books are available.

12.0 Report from Bryan Henry, Vice-President of IUPAC. For each biennium, the Vice President of IUPAC prepares an evaluation focused on a particular aspect of IUPAC activities. For 2004-2005, Prof. Henry will focus on the success or otherwise of the project system. He is visiting each of the Divisions' meetings this year in order to obtain a better knowledge of their work and their concerns and problems, including monitoring the ratio between resources and output and to repair a perceived disconnect between the administration and the bodies where the work is done. He expressed pleasure in the way that Division VIII is working. The project system is working well in all Divisions and he emphasized that the system should be used more fully to bring in more projects. He suggested that different rules for Division VIII are reasonable.

13.0 Printed and Electronic Publications. S. Heller reported on the activities of the Committee on Printed and Electronic Publications.

(1) CPEP is looking at the production workflow of PAC. The Committee feels that it needs to be more concerned about policy and design rather than statistics.

(2) Dr. Fabienne Meyers, editor of Chemistry International wants to encourage all project leaders to submit articles about their projects to CI.

14.0 Indexing of the revised Red Book and revised Blue Book.

(1) It is planned that Neil Connelly will index the Red Book. The resulting index will be available for comment.

(2) For the Blue Book, a professional indexer with a chemistry background will be sought and appropriate funding will be provided.

(3) W. Powell reported having a good experience with a professional indexer at ACS and a poor experience with indexing of the book by R. B. Fox and W. Powell. He will check with ACS Books to attempt to locate a professional indexer.

15.0 IUPAC and IUBMB Nomenclature Web Site (Queen Mary, University of London).

15.1 G. Moss distributed the latest statistics on the Queen Mary web site (see Appendix I)

15.2 Relationship with the IUPAC web site and plans for the future. Information about the iupac.org website to facilitate discussion about documenting the feasibility of hosting the Queen Mary site on the main server is given at:

http://www.rsc.org/IUPAC8/attachments/IUPACorgFacilities.pdf

15.3 There are several issues with mirroring the Queen Mary web site to the IUPAC web site.

(1) The IUPAC.org site is outdated; it was done in HTML, not in XML as would be done today.

(2) Searching is a problem; internal linking is difficult

(3) To get the same statistics now obtained from the Queen Mary site might be a problem on the IUPAC web site; at present the information from the latter might not be as useful. A list of the statistics that would be useful should be developed.

(4) The solution may be to get semi-volunteers to generate a professional IUPAC web site that IUPAC would own. Miloslav Nic and Jiri Jirat in Prague have created a new website with XML that is a possibility; the Gold Book is on this web site as well as on the present IUPAC web site.

S. Heller will put together an e-mail report to B. Henry about the IUPAC web site.

(5) To transfer the Queen Mary web site to the IUPAC web site will require the links between JCBN and IUBMB to be disentangled.

(6) S. Heller will send an e-mail to CPEP members recommending that Nic and Jirat set up and maintain the IUPAC web site with Fabienne Meyers operating the input. Cost estimates were given as: computer, $2000; set-up, $10-15000; plus annual maintenance.

16.0 Revision/Updating of Existing Recommendations.

It was agreed that the following procedure used for the Section F update was appropriate for updating existing published recommendations.

Revised Section F: Natural products and related compounds (IUPAC Recommendations 1999), *Pure Appl. Chem.* **71**, 587-643 (1999),

http://www.chem.qmul.ac.uk/iupac/sectionF/

was updated as a publication "Errata. Revised Section F: Natural products and related compounds (IUPAC Recommendations 1999). Corrections and modifications (2004)", *Pure Appl. Chem.* 76(6), 1283-1292, 2004; changes in the 1999 recommendations (the original publication) were noted as marked changes in the web publication

http://www.chem.qmul.ac.uk/iupac/sectionF/

It is planned to update "Nomenclature for the C_{60}-I_h and C_{70}-$D_{5h(6)}$ Fullerenes (IUPAC Recommendations 2002)", *Pure Appl. Chem.*, 2002, 74, 629-695,

http://www.chem.qmul.ac.uk/iupac/fullerene/

in this manner.

17.0 Standardization of expressions for names. Previously, many words and/or expressions have been used to express levels of preference of IUPAC names, for example, recommended, preferred, allowed, permitted, acceptable, legitimate, obsolescent, not encouraged, discouraged, not included, formerly named as, disallowed, and prohibited. It was agreed to aim to use only preferred, acceptable, and unacceptable in future publications.

18. Advisory Subcommittee Membership. The following were suggested as additional members: Dr. Jeffrey Wilson, Prof. Alexander Senning, Dr.Ursula Bünzli-Trepp, Dr. Libuse Goebels, and Mr. Jeff Carter to the current membership, which is given in

http://www.rsc.org/IUPAC8/attachments/DivVIIISubcomMemb.doc
http://www.rsc.org/IUPAC8/attachments/DivVIIISubcomMemb.pdf

19. Divisional National Contacts. In the Vice President's Critical Assessment at the General Assembly in Ottawa, it was proposed that all National Adhering Organizations be given the opportunity to appoint a National Contact for those Divisions on which they are not represented (see also:

http://rsc.org/IUPAC8/attachments/NationalContacts_2004.pdf)

For Division VIII such a person would be added to the Advisory Subcommittee and noted as DNC.

The Division Committee members were reminded that each member is supposed to report to his own National Adhering Organization about IUPAC activities.

20. Other business.

21.1. National Representatives. An increase the number of National Representatives from 6 to 10 was approved at Ottawa. If this is to continue, it must be added to the Rules of the Division which must be approved by the Bureau. A. McNaught has indicated to the Bureau that we will go forward with 10 National Representatives.

21.2. The next meeting of the Division Committee would be August 13-14, 2005 during the General Assembly in Beijing. Task Group meetings will precede the Division Committee meeting and there will be an Open Meeting of the Division Committee on August 12, 2005.

21.3 Task Group meetings:

(1) Structure representation, September 1-2, 2004, 9:30 a.m.

(2) Red Book Revision, September 1-2, 2004, 9:00 a.m.

(3) Rotaxanes, September 1, 2004, 3:00 p.m.

(4) Fullerenes II, September 2, 2004, 9:00 a.m.

Respectively submitted: Warren H. Powell (Secretary) 12/6/04

Accepted: Alan D. McNaught (President) 12/9/04

APPENDIX I

Nomenclature World Wide Web Database – Statistics

Statistics based on log of IP addresses used each day. Total usage to date about 3230000. Data on 182 countries recorded so far. Summary data for 1996-2003 at

www.chem.qmul.ac.uk/iupac/usage/

For full details of each document see

www.chem.qmul.ac.uk/iupac/ or www.chem.qmul.ac.uk/iubmb/

Average use **per week**

Year	1996	1997	1998	1999	2000	2001	2002	2003	2004
Total usage	296	650	1476	2786	5515	9813	15360	19105	22435
Search Facility	-	-	-	204	1663	4169	8355	11308	13680
Bibliographic Data	-	61	142	235	325	470	598	655	730
Map of Usage	-	7	8	29	37	58	83	78	93
IUPAC Nomenclature									
Class Names Glossary	138	157	430	693	1039	1504	2178	2492	3027
Physical Org Chem Glossary	29	36	136	343	751	1089	1796	1934	2207
Atomic Weight	23	48	95	144	310	651	964	1431	1587
Periodic Table	-	-	-	17	155	291	475	870	876
Stereochemical Glossary	-	32	85	135	231	392	602	694	814
Medicinal Chemistry Glossary	-	-	56	87	150	316	532	601	634
Section F (Natural Products)	-	-	-	14	121	321	450	505	591
Bioinorganic Glossary	-	-	61	108	201	391	633	570	562
Fused Ring	-	-	64	73	110	198	241	275	321
Ions and Radicals	-	-	-	-	72	150	196	226	265
Numerical Term	-	18	27	35	54	99	150	189	234
Gold Book	-	-	-	-	80	127	155	162	184
Phanes	-	-	31	42	56	80	95	135	177
Regular Organic Polymer	-	-	-	-	-	-	-	-	161
Fullerenes	-	-	-	-	-	-	69	124	161
Hantzsch Widman	12	14	31	46	56	89	116	125	150
von Baeyer	-	-	-	29	61	106	130	118	135
Spiro	-		-	26	47	90	114	115	134
Delta Convention	8	9	19	30	54	82	110	106	131
Section H (Isotopic Label)	-	-	26	34	46	73	90	93	115
Element Name > 100	-	-	-	20	45	78	87	93	114
Lambda Convention	6	8	17	28	40	60	76	74	83
Phane II	-	-	-	-	-	-	-	59	69
Guide Errata	-	-	-	20	21	25	32	47	54

IUPAC/IUBMB Nomenclature

Carbohydrates	46	72	144	237	453	835	1156	1444	1721
Amino Acids & Peptides	31	62	135	186	359	670	1072	1366	1553
Steroids	12	21	87	93	396	811	1213	1460	1287
Vitamin D	-	-	-	-	47	69	125	209	364
Vitamin B-6	-	-	-	34	95	155	267	466	363
Vitamin B-12	-	-	-	49	69	146	266	315	323
Folic acid	-	-	-	60	58	210	208	304	306
Tocopherol	-	-	21	33	48	80	150	274	274
Lipids	-	-	-	29	70	132	198	232	272
Nucleic Acid Abbreviations	-	-	-	45	77	136	202	241	260
Tetrapyrroles	-	-	-	-	-	124	221	227	260
Glycolipids	-	-	15	35	65	91	137	171	209
Glycoproteins	-	-	20	32	71	134	172	187	188
Cyclitols	-	-	21	51	72	113	174	178	184
Lignans and Neolignans	-	-	-	-	-	71	123	137	177
Polypeptide Conformation	-	8	14	34	61	111	173	191	174
Carotenoids	-	-	-	-	46	84	128	148	174
Polysaccharide Conformation	-	8	14	26	49	82	134	153	160
Biochemical Phosphorus	-	-	-	-	62	103	151	147	144
Retinoids	-	-	-	-	35	71	99	126	144
Polynucleotide Conformation	-	7	15	27	44	68	92	103	120
Quinones with Isoprenoid Chain	-	-	-	-	-	47	90	105	119
Polymerised Peptides	-	-	-	-	34	56	91	97	111
Prenols	-	-	-	19	33	55	77	84	100

	1996	1997	1998	1999	2000	2001	2002	2003	max
Both Committees									
Committees' Homepage	18	38	65	123	268	423	653	801	1043
Newsletter	-	-	25	59	145	304	456	446	585
IUBMB Nomenclature									
Enzymes	16	54	124	320	1086	2088	3560	4260	5536
EC 1	-	-	-	35	241	487	922	1091	1437
EC 2	-	-	-	-	180	438	769	900	1162
EC 3	-	-	-	-	165	427	947	1054	1456
EC 3.4 (50 file)	16	54	>82	200	285	281	184	114	120
EC 3.4 (single)	-	-	-	-	-	134	343	397	552
EC 3.4 (total)	-	-	-	-	-	336	484	472	629
EC 4	-	-	-	-	90	223	410	423	556
EC 5	-	-	-	-	64	164	294	322	425
EC 6	-	-	-	-	46	138	239	261	309
reaction	-	-	-	-	48	119	381	650	994

newenz	-	-	-	-	53	60	75	71	77
Enzyme Supplement 5	-	-	42	66	79	53	37	29	31
Enzyme Kinetics	-	-	16	61	152	249	365	441	569
Membrane Transport Proteins	-	-	-	-	-	-	93	157	183
Electron Transport Proteins	-	-	-	-	58	107	163	165	180
Biochemical Thermodynamics	-	-	22	40	66	107	132	148	174
Incomplete Nuc. Acid Sequence	-	9	20	31	50	75	103	137	170
Isoenzymes	-	-	14	28	68	106	124	123	149
myo-inositol	-	-	11	23	43	74	125	125	124
Peptide Hormones	-	-	-	-	32	51	80	101	118
Branched Chain Nucleic Acids	-	3	6	10	40	63	115	107	99
Multienzymes	-	-	10	13	18	25	37	36	43
Translation Factors	-	-	-	-	11	18	34	37	39

GPM
28 April 2004