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

Beijing, China, August 13-14, 2005

Members present: Mr Jonathan Brecher, Dr Ture Damhus, Prof Richard Hartshorn, Dr Stephen Heller, Dr Michael Hess**,** Prof Jaroslav Kahovec, Prof G Jeffrey Leigh**,** 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 David StC Black (IUPAC Secretary General)

National Representatives Present: Prof Jan Reedijk (Netherlands), Dr. Paolo Righi (Italy)

Observers: Dr. David Barden (RSC Young Observer), Dr Karl-Heinz Hellwich (elected Titular Member for 2006), Dr William Town, in part (Project Leader, Graphical Representation Standards)

Members Absent (excused): Prof Herbert Kaesz, Prof Dr Alexander J. Lawson, Dr Antony Williams

The fifth meeting of the Division Committee of the IUPAC Division of Chemical Nomenclature and Structure Representation at the Beijing International Convention Center was convened by President McNaught at 9:00 a.m. on Saturday, August 13, 2005.

1.0 President McNaught welcomed the members to this meeting and offered a special welcome to the National Representatives, Prof Jan Reedijk (Netherlands) and Dr Paolo Righi (Italy): to Dr David Barden, a Young Observer from the Royal Society of Chemistry; and to Dr Karl-Heinz Hellwich, an elected Titular Member for 2006. He also noted that Prof Herbert Kaesz, Prof Dr Alexander J. Lawson, and Dr Antony Williams would be unable to be with us. It was noted that Prof David Black, the IUPAC Secretary General, would be visiting during the meetings and that Dr Peter Atkins, Chairman of the IUPAC Committee on Chemical Education, would join our meeting at some point. Each of the attendees introduced himself and provided some background information. Housekeeping details regarding breaks and lunch were announced.

2.0 The agenda as circulated was approved with the addition of the following topics:

Cross representation on other international bodies (minute 13.0).
Elections (minute 9.5)
Translations of IUPAC recommendations (minute 14.0)
The IUPACVIII Webboard (hosted by RSC) (minute 13.2)

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/DivisionCommitteeMinutesBudapestFinal.rtf
http://www.rsc.org/IUPAC8/attachments/DivisionCommitteeMinutesBudapestFinal.pdf

were approved with the following correction.

3.1 Item 7.3 (2) should read “Dr Damhus submitted examples to try to coordinate the use of the multiplicative prefixes 'di, tri, ...' vs. 'bis, tris, ...' between the revised Blue Book and the soon to be published Red Book.

4.0. Matters arising from the Budapest minutes.

4.1. It was noted that the document ‘Graphical Representation of Stereochemical Configuration’ uses ‘not acceptable’ rather than ‘unacceptable’ as given in item 17.0 of the Budapest minutes. It was agreed that this usage should be retained.

5.0. Report from the meeting of the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) in Columbia, Missouri on April 30th and May 1st 2005.

The minutes of the meeting of the Nomenclature Committee of IUBMB (NC-IUBMB) and the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) held in Columbia, MO, USA on April 30-May 1, 2005 may be found at:

http://www.rsc.org/IUPAC8/attachments/JCBN_minutes_Columbia_2005(draft).pdf

Dr Moss noted that the meeting in Columbia, MO was concerned mostly with enzymes.

Dr. McNaught reported that the enzyme information database BRENDA now uses InChI.

Developing projects in IUPAC-IUBMB that will require IUPAC approval:

(1) An addendum to the 1996 carbohydrate nomenclature, to include areas not well covered in that document.

(2) A revision of the old JCBN document on Phosphorus-Containing Compounds of Biochemical Importance (Eur. J. Biochem. **1977**, *79*, 1-9; Biochemical Nomenclature and Related Documents, 1992, pp. 256-265)

(3) Compilation of a list of biochemical compounds that are not a part of any other IUPAC-IUBMB documents and for which advice is needed.

Membership: Prof Dietmar Schomburg was appointed as Chairman (funded by IUBMB) and Prof Sinéad Boyce reappointed as Secretary (funded by IUBMB). Prof Richard Cammack will serve as Past Chairman and Treasurer. Prof J. F. G. Vliegenthart (IUBMB) and Dr Gerry Moss (IUPAC) were reappointed to four-year terms. The Division VIII Committee endorsed these appointments.

6.0 Publications since the 2004 meeting in Budapest:

6.1 Numbering of Fullerenes, *Pure Appl. Chem*, **2005**, ***77***, 801-923:

http://www.iupac.org/publications/pac/2005/7705/7705x0843.html

There were 200 reprints of this publication sent to Dr Powell. This seems far to many in this age when copies are so readily available on line. This needs to be discussed by the Publications Committee.

6.2 "International chemical identifier goes online", *Chem. World*, **2005**, ***6***, 7:

http://www.rsc.org/chemistryworld/Issues/2005/June/International_chemical_identifier.asp

6.3 In the July-August issue of *Chem. Int.* there is an article about the treatment of element names in the new edition of the "Red Book" by P. Goya and P. Román specifically titled "Wolfram vs. Tungsten", along with a reply from Dr Ture Damhus on behalf of the editors of the 2005 "Red Book". This may be found at:

http://www.iupac.org/publications/ci/2005/2704/ud_goya.html

It was noted that there are numerous differences in naming and/or spelling of element names for nationalities other than English. Footnotes and explanations, which are often very useful, are often provided in papers but not in books

7.0 Division VIII Projects:

7.1 IUPAC International Chemical Identifier (InChI) (Dr Steve Heller)

The IUPAC International Chemical Identifier (InChI) is a protocol for converting a chemical structure (connection table) to a unique, predictable ASCII character string. Version 1.0 of the Identifier released in April 2005 expresses chemical structures in a standard machine-readable format, in terms of atomic connectivity, tautomeric state, isotopes, stereochemistry, and electronic charge. It deals with neutral and ionic well-defined, covalently-bonded organic molecules, and also with inorganic, organometallic and coordination compounds. Software, documentation, source code, and licensing conditions are available from the IUPAC website at:

http://www.iupac.org/inchi

An InChI frequently asked questions (FAQ) by Nick Day (Unilever Centre for Molecular Informatics, Cambridge University) is available from:

http://wwmm.ch.cam.ac.uk/inchifaq/

A full publication of the InChI protocol probably will appear in a NIST journal within the next year.

A new project, titled "IUPAC International Chemical Identifier (InChI): Promotion and Extension (2004-039-1-800)" has been established to promote the use of the Identifier throughout the chemical information community; to extend its applicability to include polymeric structures; to explore the need for other extensions, including the ability to handle Markush structures; and to include information on other attributes, such as phases and excited states. For additional information see:

http://www.iupac.org/projects/2004/2004-039-1-800.html
http://webboard.rsc.org:8088/~INCHI-L

It was suggested that InChI be publicized outside of information circles.

To enable development of InChI facilities and applications in an Open Source context, a project to encompass this work has been registered with SourceForge.net (see http://sourceforge.net/projects/inchi); anyone wishing to participate should contact the project administrator (mcnaughta@rsc.org) or the IUPAC Secretariat (secretariat@iupac.org). To receive and discuss proposals for InChI enhancements, an Internet listserver has also been established; anyone wishing to participate in these discussions should contact Dr Alan McNaught (mcnaughta@rsc.org).

There are two problems that must be recognized. One is related to chemistry, i.e., how the structure is drawn, for example, tautomers. The other is interpretation by the chemist. An InChI cannot be derived if the structure cannot be accurately drawn or can be represented as a molfile; InChI is based on molfile. InChI must support many formats, included disconnected diagrams. It is necessary to be able to verify that the output from an InChI is the same as the input.

Although in principle publishers could probably derive InChIs more easily than authors, publishers may not be willing to take on the extra work and may leave the responsibility for InChI generation to the authors.

In May, 2005, ACD Labs announced that they would be fully implementing the InChI protocol into their structure drawing program ACD/ChemSketch. U.S. Patent Office is interested in InChI. The European Patent Office expressed interest one and a half years ago, but nothing has developed yet.

CAS is looking into various formats and doesn't see InChI being used in its products today. Beilstein is considering InChI and seems to like it, but management has yet to be convinced.

InChI has been adopted by the National Institute of Standards and Technology (NIST)(150,000 structures); the National Institutes of Health/National Centre for Biotechnology Information (NIH/NCBI)/PubChem (3 million+ structures; the National Cancer Institute (NCI) Database (23 million+ structures; the Environmental Protection Agency Distributed Structure-Searchable Toxicity (EPA DSSTox) Database (1450 structures); the Kyoto Encyclopedia of Genes and Genomes (KEGG) Database (9584 structures); the University of California at San Francisco ZINC Is Not Commercial Database (UCSF ZINC) (3.3 million structures.

InChIs can be searched in Google.

A list of talks about InChI given in 2005 appears in Appendix I. After they are actually given they will be available on Dr Steve Heller's website (http://www.hellers.com/steve/pub-talks/)

Appendix II gives a list of InChI references and/or publications.

7.2 Preferred names in the nomenclature of organic compounds: new Blue Book (Dr Warren Powell)

The revised "Nomenclature of Organic Chemistry", a more comprehensive set of recommendations than has ever been attempted previously and which contains recommendations for selecting preferred IUPAC names (PINs), was submitted for public and ICTNS review last fall. The deadline for comments was set at March 31, 2005. A number of comments and suggestions were submitted to the Division's Webboard before the deadline, dealing with topics such as proper use of 'di-', "tri-", etc. *vs*. "bis-", "tris-", etc: enclosing marks, amine oxides, acid esters, compound locants, adducts. Consideration of these items was started immediately, i.e., before the deadline for comments. Comprehensive sets of comments were received from U. Buenzli-Trepp, and G. Eller. Comments or other contributions were also received from G. Moss, T. Damhus, E. Godly, J. Brecher, L. Maat, J. Nyitrai, K-H. Hellwich, R. Sayle, R. Cammack, J. Wilson, A. Yerin, R. H. de Rossi, J. Reedijk, B. Herold,

H. Schepers, J. Kahovec, A. Senning, H. Dixon, H. Gottlieb, L. Salvetella, M. Ennis, R. Hartshorn, and P. Mata,

Prof Favre, Dr Powell, and Dr McNaught met in Boston April 25-28, 2005 to evaluate all the comments received to date and to prepare for appropriate revisions to the September, 2004 manuscript.

At the present time, Chapter 1 has been revised (sections on multiplicative nomenclature, functional class nomenclature, and adducts are not yet incorporated) and Chapters 2, 9, and 10 have been revised. Major revisions are still to be incorporated in Chapters 3-6. Comments on Chapters 7-8 have still to be evaluated. There are enough significant revisions to the manuscript that it may be necessary to undergo further reviews. A real problem is how to do reviews of such an extensive manuscript thoroughly, but efficiently. There are few people willing to tackle the entire work. Perhaps it could be divided among several reviewers, but this raises questions of consistency between sections.

7.3 Nomenclature of inorganic chemistry: revision of the Red Book (Dr Ture Damhus)

The task group for revision of "Nomenclature of Inorganic Chemistry" (the Red Book) is waiting for a second page proof after which Prof N. Connelly will prepare the index. There will not be time to review the index as was suggested in Budapest. It was noted that the index to the 1990 edition as prepared by Blackwell Science was deemed not adequate by a number of readers. Dr Hellwich volunteered to look over the index if it would fit into his available time.

7.4 Rotaxanes (Project 2002-007-1-800; Dr Andrey Yerin)

Comments and proposals sent via e-mail by Edward Wilks and Jaroslav Kahovec were considered at a meeting of the project group in Budapest (August 2004). Since several comments complained that the document is very difficult for chemists not so experienced in nomenclature, it was decided to separate the document into two different parts: (1) general rotaxane nomenclature and (2) designation of configuration in rotaxanes. Because of this general change most topics had to be reformulated.

The next version of the document (Version D) was distributed to the project group members at the beginning of July, 2005. Approval of Version D and consideration of comments from Dr Metanomski are scheduled for the Beijing meeting of the project group on August 10, 2005, after which the document can be made available for public review.

Assuming that all main terms and procedures of rotaxane nomenclature are covered by this project, the preparation of a new draft document on Nomenclature for Macromolecular Rotaxanes is planned (see minute 7.6.3)

7.5 Extension of IUPAC rules for stereodescriptors to coordination numbers 7-12 (Project 2003-025-1; Prof G. Jeffery Leigh)

A project task group was established in Budapest to evaluate procedures for describing geometry of coordination polyhedra with coordination numbers 7 through 12. A final report of this project can be found on the Division VIII webboard under General messages.

http//www.webboard.rsc.org/IUPACVIII

A Technical Report based on this report is in preparation.

The main problem in describing the stereochemistry of coordination polyhedra is recognition of a discrete polyhedron because of distortion. This problem becomes more difficult as the number of coordination sites increases. The report recommends that IUPAC endorse the method of Dr T. E. Sloan, et. al., for all recognized coordination numbers up to and including coordination number 7 and be extended to include specific examples that are deemed reliable for coordination numbers 8 and 9.

7.6 Macromolecular projects (with Division IV)

A general progress report from Michael Hess can be found at:

http://www.rsc.org/IUPAC8/attachments/Hess_Report_2005_DivVIII.pdf

The next edition of the "Compendium of Macromolecular Nomenclature" should be published next year. Dr Metanomski and Dr Wilks are giving it a final check. It is a compilation of already published material and will not be subjected to the full formal review processes. It was noted that the names in the older chapters are not in conformity with the 1993 Guide to IUPAC Nomenclature of Organic Compounds.

A feasibility study of a project on abbreviations is being considered.

7.6.1 Source-Based nomenclature of Single-Strand Organic Polymers (2003-042-1-800)
Task group Leader: T. Kitayama

This is an ongoing project.

7.6.2 Source Based Nomenclature for Modified Polymer Molecules (1999-051-1-800)
Task Group Leader: T. Kitayama

This is an ongoing project.

7.63 Nomenclature for (Macromolecular) Rotaxanes (2000-037-1-800)
Task Group Leader: A. Yerin

Work on the document "Nomenclature for Macromolecular Rotaxanes" was stopped at the Ottawa meeting in 2003 because of the project "Nomenclature for Rotaxanes" (2002-007-1-800) which was devised to develop general principles for nomenclature of rotaxanes not containing macromolecular units. Now that this latter project is almost finished and all main principles of rotaxane nomenclature are agreed, the work on recommendations for nomenclature of rotaxanes containing macromolecular units can continue. All changes necessary to follow the developed principles for naming low molecular mass rotaxanes will applied.

The latest available draft of Nomenclature for Macromolecular Rotaxanes is dated 2003 and includes comments sent for the meeting of the task group in Ottawa. As all main definitions are already included in the low molecular mass rotaxanes document, the 2003 draft on macromolecular rotaxane nomenclature can be reduced and will deal only with the macromolecular parts of rotaxane nomenclature.

Discussion of the work needed to finish the recommendations for macromolecular rotaxane nomenclature is scheduled for the meeting of the rotaxane project group

(2002-007-1-800) here in Beijing on August 10th 2005; consultation with Division IV is needed.

7.6.4 Terminology and Structure-Based Nomenclature of Dendritic and Hyperbranched Polymers (2000-081-1-800); Task Group Leader: J. Kahovec

The next steps will be expert review followed by public and ICTNS review. A list of reviewers is still needed. Dr Karl-Heinz Hellwich noted that there is still a problem of consistency with general terms.

7.6.5 Terminology and Nomenclature of Macromolecules with Cyclic Structures (2000-082-1-800); Task Group Leader: W. Mormann

Completed subject to approval by the task group here at the Beijing meeting.

7.7 Cyclic peptides (Dr Gerard Moss)

The document "Nomenclature of Cyclic Peptides (Recommendations, 2004)" has been through both public and ICTNS review. Several issues, mostly of a biochemical nature, need to be settled. The main problem is the use of the term 'cyclo' in a way that is not consistent with its use in natural products nomenclature. Publication will probably occur later in 2005.

7.8 Graphical representation standards for chemical structure diagrams (Dr Jonathan Brecher)

Since the meeting of the Division Committee in Budapest (2004), the comprehensive set of recommendations "Graphical Representation of Configuration" recently completed public and ICTNS review. Feedback from external reviewers and ICTNS members was very useful but did not contain fundamental criticisms. A small number of remaining issues were discussed and resolved during the meeting of the project task group here in Beijing. It is expected that these recommendations will be ready for publication very soon, once the conclusions reached by the project task group are transcribed into the final document.

The project task group has also started work on the second part of its responsibility, i.e., a document containing recommendations for all other (non-stereochemical) aspects of graphical structure representation. Significant work has been completed on that document titled "Graphical Representation Standards for Chemical Structure Diagrams"; it is already one-third longer than the document on recommendations for configuration discussed above. Some of the remaining issues slated for inclusion in this document were discussed by the project task group in Beijing, but others remain to be considered. It is hoped that this document will be ready for public and ICTNS review during the first half of 2006.

In light of rapid progress in both of these areas, it has proven too difficult to keep the html version of the two documents in sync with the pdf version. Accordingly, the html version that was formerly posted at angelfire.com is no longer available. The pdf version is being circulated among members of the working party periodically as changes are made, and could be provided to other interested parties if there is concern about the loss of the html version.

7.9 Comparison of procedures for naming hydro derivatives of fused ring systems (Dr Warren Powell)

As noted in minutes of the meeting of the Division Committee in Budapest (minute 7.11) the 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 recommendations by the IUPAC Commission on Nomenclature of Organic Chemistry, but now planned as a technical report, was sent to Dr Karl-Heinz Hellwich and Dr Jeffrey Wilson for review of the respective Beilstein and CAS procedures. Their comments and corrections have been received but have not yet been incorporated into the document.

It was noted that an example reflecting this comparison should be added to the new Blue Book in an appropriate Section. It was also noted that Beilstein's AUTONOM will follow the IUPAC recommendations.

Although not yet public, the URL for this document is:

http://www.chem.qmul.ac.uk./iupac/misc/hydro.html

8.0 Future Projects

8.1 Preferred names for inorganic compounds (Dr Ture Damhus)

A meeting of those who had expressed an interest to Dr Damhaus in a project to develop preferred names for inorganic compounds was held in Budapest. The report of this meeting is given as Appendix III. Because of commitments to the revised Red Book, to ICTNS, and other projects, Dr Damhaus was unable to prepare a project proposal and will not be able to lead such a project. Hence, a steering group consisting of Prof R. Hartshorn, Prof J. Reedijk, Prof J. Leigh, and Dr T. Damhus was formed to develop a proposal for work on preferred names for inorganic compounds. A place and time for a meeting was to be discussed.

8.2 Metallacycles (Warren Powell)

A project proposal is being developed by Prof. H. Kaesz and Dr W. Powell based primarily on a previous report by Prof H. Kaesz, Mr J. Casey, Prof H. Favre, and Prof Y. Yamamoto entitled "Nomenclature of Metallacycles of the Transition Metals**"** dated June 25, 2001. It was noted that Dr A. Hutton and Prof E. Nordlander should be a part of this project. The scope of the project was said to be too broad; the 'ocene' type of compound should not be included but should be a separate project. Dr McNaught would write to H. Kaesz about this.

8.3 Adducts (Dr Warren Powell/Dr Ture Damhus)

In response to requests mainly from the project group for the revised Red Book, consideration has been given to adding a subsection to the new Blue Book to deal with addition compounds, other than those involving boron compounds as given in Section P-68.1. A proposed subsection (P-14.7) can be found on the Webboard:

http//www.webboard.rsc.org/IUPACVIII

For inorganic compounds, the revised Red Book recommends that the name be based on the order of citation of components in the structure, which is based first on the increasing number of each component and then alphabetically.

Although the 'inorganic' method may work for inorganic compounds, there can be problems when applied to organic compounds. The proposed subsection P-14.7 orders the components according to the hierarchy used in organic nomenclature as given in subsection P-41 of the new Blue Book. This method is very similar to the 'compd.

with' method used by CAS. Hierarchical arrangement permits similar names for compounds differing only in the ratio of components.

It was noted that the method used in organic recommendations involving the use of parenthetical element symbols connected by a long dash to indicate a coordinate bond between the named elements should be contrasted with the method of coordination compounds; the latter seemed much more rational and easier to apply.

It was recommended that Meisenheimer complexes be removed from the proposed subsection P-14.7.

It was agreed that further consideration of this subject be carried out by a small group consisting of Dr K-H. Hellwich, Dr A. Yerin, Dr T. Damhus, and Dr W. Powell.

8.4 Preferred structure-based names for macromolecules

As soon as the final draft of the new Blue Book is finished, it will be necessary to evaluate its consequences for macromolecular nomenclature with a view to preferred structure-based names for macromolecules.

8.5 Boron nomenclature

Correspondence with Dr John Kennedy has indicated that he does not wish to lead a project on boron nomenclature. It was suggested to send a representative to the next IUPAC Boron Conference to try to find interest.

8.6 Other future projects

8.6.1 A second edition of the book "Principles and Practices of Chemical Nomenclature, A Guide to IUPAC Recommendations" published in 1998, authored by G. J. Leigh, H. A. Favre, and W. V. Metanomski.

> [Secretary's note: Subsequent to the meeting, it was learned that according to the Secretariat's records, Blackwell has sold 1369 copies and the Secretariat has sold 116 for a total of 1485 The list price is USD 30. There are 16 copies left in stock. About 20 copies have been given away over the years at conferences, etc.

Prof G. J. Leigh is willing to organize such a project. Planning should take a year with actual work starting in 2006. Dr Hellwich volunteered to be involved. Suggestions as to content should be sent to Prof Leigh.

Content should include an emphasis on decoding names as well as coding them. Perhaps a list of abandoned trivial or common names and their systematic equivalents should be included. A historical introduction might be included.

8.6.2 Stereochemical nomenclature.

Chapter 9 in the new Blue Book describes, in detail, the use of descriptors in names. Description of configuration in coordination complexes with higher coordination numbers has been studied (see minute 7.5). Perhaps it is time for a full discussion of the principles of stereochemical nomenclature for both organic and coordination structures in a separate book.

Dr K.-H. Hellwich has proposed a project on conformation stereochemistry, but so far there has been no interest expressed.

The need to revisit stereochemical terminology should be examined.

8.6.3. Ambiguity in Names.

It was noted that there was a meeting at 4:00 p.m. today in Hall 10 in the Beijing International Convention Center to discuss ambiguous terminology in chemical names. Dr K.-H. Hellwich will attend.

8.6.4 Problems of those dealing with chemical names who know nothing about chemistry or nomenclature. Dr David Barden noted that Aldrich was used as an "authority" on nomenclature by at least some laboratories.

9.0 Committee Membership

9.1 Election of Titular Members has been completed. Dr G. P. Moss will continue as a Titular Member and assume the office of President. Dr A. D. McNaught will continue as a Titular Member and assume the position of Past-President. Dr W. H. Powell was elected for a further two-year term as a Titular member and Secretary. Drs Steve Heller and K.-H. Hellwich were elected as Titular Members for four year terms.

The complete list of Titular Members is thus as follows:

Dr Gerry Moss (President)
Dr Warren Powell (Secretary)
Dr Alan McNaught (Past President)
Dr Ture Damhus
Prof Richard Hartshorn
Dr Steve Heller
Dr Karl-Heinz Hellwich
Dr Jaroslav Kahovec
Prof Joszef Nyitrai
Dr Andrey Yerin

9.1 Associate Members 2006-2007. The following was approved by the Division Committee in Beijing.

Mr Jonathan Brecher and Prof. G. J. Leigh will continue as Associate Members. Prof R. G. Jones, Dr J. Wilson, Dr A. T. Hutton, and Prof. F Cozzi were nominated as Associate Members and will be contacted concerning their willingness to accept this position. Assuming that the above four will accept their positions, the complete list of Associate Members will be as follows:

Mr Jonathan Brecher
Prof Franco Cozzi
Dr Alan T. Hutton
Prof Richard G. Jones
Prof. G. Jeffery Leigh
Dr Jeff Wilson

9.2 National Representatives 2006-2007. The current number of National Representatives is 9; we are allowed 10 according to the modification of the Division Rules (see Appendix VI) approved for the Budapest meeting (see minute 20.1 in the Budapest meeting). Three current National representatives cannot be reappointed as they have reached their maximum years of service. The National representative from Argentina, Prof Rita Hoyos de Rossi, cannot be reappointed because Argentina has not paid its dues. Five National Adhering Organizations have nominated representatives. Hence, we have the following new National Representatives:

Prof Ivan Dukov (Bulgaria)
Prof S S Krishnamurthy (India)
Prof Youngkyo Do (Korea)
Dr Farzana Ansari (Pakistan)
Prof Martin Putala (Slovakia)

The list of reappointed National Representatives for 2005-2007 is as follows.

Prof Len Lindoy (Australia)
Dr Martin Ragnar (Sweden)
Prof Jan Reedijk (Netherlands)
Dr Paolo Righi (Italy)

[Secretary's note: Subsequent to the meeting it was learned that Argentina has paid it dues an therefore Prof Rita Hoyos de Rossi will be the National Representative from Argentina for 2005-2007]

9.3 Vice-President: procedure for election

It was agreed that the Division Committee should always retain three officers, President, Secretary, and Past President OR President, Secretary, and Vice-President. Since we have the office of Past-President this year, an election of a Vice-President is not urgent and should be further considered at next year's meeting

9.4 Advisory Subcommittee 2006-2007. The current list of members of the Division VIII Advisory Subcommittee is given in Appendix IV. The following were nominated as new members. They will be contacted to be sure that they are interested in joining the Advisory Subcommittee.

Mr Thomas E. Sloan
Dr Robert Temme
Dr Kirill Degtyarenko
Dr Harry Gottlieb
Dr Elizabeth Weber

9.5 Election procedure

Because the procedure used for the Division VIII elections this year had been questioned, it was felt necessary that it be reviewed. The procedure for Division Elections is included as items 4-6 of the Division Rules of the Chemical Nomenclature and Structure Representation Division given in Appendix V.

Dr G. J. Leigh explained his objections to the procedure used for the 2005 elections and Dr G. P. Moss, who was the Chairman of the Nominating Committee for the 2005 elections, detailed the procedure that was used.

It was noted that there were necessary differences for Division VIII Committee elections from other Divisions, mainly which in addition to geographical constraints, the Division VIII Committee must possess acceptable knowledge of the whole range of nomenclature and cognate disciplines.

It was agreed to have a full discussion about the nominating procedure at the Division VIII meeting next year. The following suggestions were offered.

- Be more active in encouraging applications for the "young observers" program.
- Have data on the members whose terms are expiring available before the meeting in Prague.
- Provide more candidates for consideration.

10.0 Publicity

A publicity plan to be implemented when the new Red and Blue Books become available as noted in the Budapest minutes was still to be prepared. Publicity for the IUPAC colour books by RSC will no doubt be no more than that provided for other books published by RSC. Dr A. McNaught will try to generate a plan for publicity. Previous minutes contain lists of suggestions for methods of publicizing the work of Division VIII.

ACS Career Workshops had been successfully run in collaboration with other IUPAC Divisions but don't seem appropriate for Division VIII.

Other suggestions for publicity included:

(1) Build ways to highlight nomenclature matters in the new IUPAC website.

(2) Press releases about new colour books or new editions of nomenclature manuals.

(3) New book announcements in chemistry journals.

(4) Book reviews

(5) Publications on nomenclature problems and pitfalls.

(6) Letters and/or notes on nomenclature matters in journals.

11.0 Article for Chemistry International

Dr F. Meyers has requested a one page report on what Division VIII accomplished here in Beijing for publication in *Chemistry International* this fall.

12.0 Report from the Committee on Printed and Electronic Publications (Dr Steve Heller)

The IUPAC website is moving from Research Triangle Park (RTP) to the Fachinformationszentrum (FIZ) Berlin which is donating two servers to IUPAC. The move will occur in a three-step migration and duplicate sites will coexist for a while before the move is complete. The purpose of developing a new IUPAC website is to incorporate the Division VIII Webboard (now located on the RSC website) and the IUPAC and IUBMB Nomenclature Web Site (now located at Queen Mary College of the University of London

and managed by Dr G. Moss). The work is being done under contract by a group in Prague. The Prague group has converted the IUPAC website to XML. Development of the IUPAC website is a major objective of CPEP.

13.0 IUPAC and IUBMB Nomenclature Web Site (Queen Mary, University of London)(Dr Gerry Moss)

13.1. Access statistics. The statistics on the use of the website are given in Appendix VI.

13.2. There have been problems with the old software used for the RSC website during the past year which affected the Division VIII webboard. New software has been installed.

13.3 Relationship with the IUPAC web site, and plans for the future.

The new IUPAC website must be developed before the IUPAC and IUBMB Nomenclature Web Site at Queen Mary can be incorporated. Dr Moss wants to be able to develop statistics from the IUPAC website just as he does now from the IUPAC/IUBMB website.

The mirror sites for the IUPAC/IUBMB website are not necessarily kept up-to-date.

14.0 Translations

Dr K.-H. Hellwich noted that *Angewandte Chemie* has had a policy to translate IUPAC Recommendations into German, but this has turned out to be a large task. A group of translators is needed to do this. A list of German translations of IUPAC recommendations is given in Appendix VII. Translations are quite valuable as many corrections and necessary modifications to the official IUPAC English publication may emerge. These corrections can be made to the online version but a printed correction or corrigenda may be necessary as well. This has already happened with the 1993 Guide to Nomenclature of Organic Compounds and with Natural Products (revised Section F of the 1979 Organic Recommendations); in both cases printed corrections have been published. And it is happening with both publications on fullerene nomenclature.

Project groups need to be very diligent in proofing their publications to minimize corrections and editorial modifications.

The Division must alert National Adhering Organizations (NAO's) about the publication of nomenclature recommendations and ask if translations are likely. NAO's should be encouraged to translate nomenclature recommendations. The difference between translations and interpretations must be recognized. Translations need approval by the appropriate NAO.

It was suggested that a publication for *Chem. Int.* about translations could be useful.

14.0 Cross representation from the Division VIII Committee to other IUPAC Committees

14.1 Committee on Chemistry Education (CCE). Dr T. Damhus will attend the meeting of CCE here in Beijing this year. Prof R. Hartshorn will be Division VIII's representative starting next year.

14.2 Committee on Printed and Electronic Publications (CPEP). As a member of CPEP, Dr S. Heller will serve as Division VIII's representative

14.3 Committee on Chemistry and Industry (COCI). At present Division VIII does not have a representative on this committee. Dr A. McNaught will attend this committee's meeting this year here in Beijing and will attend its meeting next year if no one else is willing.

14.4. PAC Editorial Board. Dr A. McNaught will attend the meeting of this committee this year here in Beijing and will carry on to succeeding years if appropriate.

14.5. Interdivisional Committee on Terminology, Nomenclature, and Symbols (ICTNS). Dr A. McNaught will replace Dr W. V. Metanomski as a Titular Member. Prof J. Nyitrai will be Division VIII's representative. Prof J Kahovec currently represents Division IV (Macromolecular Chemistry). Dr T. Damhus remains as a Titular Member.

15.0 Next meeting

Prof J. Kahovec invited the Division VIII Committee to meet next year (2006) at the Institute of Macromolecular Chemistry in Prague. The proposed schedule was to have meetings of Project Task Groups on September 4-5, 2006 and the meeting of the Division Committee on September 6-7, 2006. These dates must still be confirmed by Prof Kahovec.

Respectively Submitted: Warren H. Powell (Secretary) 11/25/05

Accepted: Alan D. NcNaught (President) 11/30/05

APPENDIX I

Talks on InChI given by Steve Heller in 2005

1. PittCon

   "The IUPAC International Project - InChI. An Open Source/Open Access Project - March 2005"

2. ACS - San Diego (Chemical Information - Open Access session)

   "The Perfect Storm - Electronic Publishing and the Internet - March 2005"

3. 7th ICCS -International Conference on Chemical Structures - Noordwijkerhout

   "An Open Source/Open Access and the IUPAC International Chemical Identifier - InChI - June 2005"

4. 4th US Government Chemical Databases Meeting, Frederick MD - July 2005

   "The IUPAC International Chemical Identifier"

5. IUPAC 40th Congress - Beijing

   "Open Access/ Open Source and the IUPAC International Chemical Identifier (InChI) - August 2005"

6. ACS - Washington – DC (Chemical Information - Chemical Information and International Science Issues session)

   "Open Access/ Open Source and the IUPAC International Chemical Identifier - August 2005"

7. German Conference on Chemoinformatics of the German Chemical Society (GDCh - Goslar

   "Open Access/ Open Source and the IUPAC International Chemical Identifier (InChI) - November 2005"

8.PacificChem - Honolulu

   "Open Access/ Open Source and the IUPAC International Chemical Identifier (InChI) - December 2005"

APPENDIX II

List of InChI References/Publications

1. "International chemical identifier goes online", *Chem. World*, 16 May 2005

2. "Application of InChI to Curate, Index, and Query 3-D Structures, M.D. Prasanna, J. Vondrasek, A. Wlodawer and T.N. Bhat, *Proteins: Structure, Function, and Bioinformatics*, **2005**, *60*, 1-4

3. "Enhancement of the chemical semantic web through the use of InChI identifiers", S.J. Coles, N.E. Day, P. Murray-Rust, H.S. Rzepa and Y. Zhang, *Org. Biomol. Chem*., **2005**, *3*(10), 1832-1834.

4. "InChI FAQ", Nick Day (Unilever Centre for Molecular Informatics, Cambridge University): http://wwmm.ch.cam.ac.uk/inchifaq/

5. "Representation and Use of Chemistry in the Global Electronic Age", P. Murray-Rust, H.S. Rzepa, S.M. Tyrrell and Y. Zhang, *Org. Biomol. Chem*., **2004**, 3192-3203 [www.ch.ic.ac.uk/rzepa/obc/]

6. "That INChI feeling", *Reactive Reports*, Sept. 2004, issue 40.

7. "Unique labels for compounds", *Chem. Eng. News*, 2 Dec 2002

8. "Chemists synthesize a single naming system", *Nature*, 23 May 2002

9. "That IChI feeling" *The Alchemist*, 24 Apr 2002

10. "What's in a Name?" *The Alchemist*, 21 Mar 2002

11. "An Open Standard for Chemical Structure Representation: The IUPAC Chemical Identifier", Stephen E. Stein, Stephen R. Heller, and Dmitrii Tchekhovskoi, in: *Proceedings of the 2003 International Chemical Information Conference (Nimes), Infonortics*, pp. 131-143.

APPENDIX III

Exploratory meeting on a possible project on PINs (preferred IUPAC names) for inorganic compounds

Hotel Gellért, Budapest, August 29, 2004

The meeting had been convened by Ture Damhus after consultation with IUPAC colleagues on how to best probe the idea of a project on inorganic PINs and, if deemed desirable, how to get the project started.

Attendees

[Current IUPAC involvement and coordinates mentioned in the *IUPAC Handbook* are not always reproduced here.]

Dr. Piroska Fodor-Csanyi (Hungary) is an inorganic and physical chemist and radiochemist. Dr. Fodor-Csanyi has been involved in nomenclature work since the early sixties, has been on the former IUPAC Commission on Nomenclature of Inorganic Chemistry (CNIC) and has in particular contributed with translations of IUPAC rules into Hungarian.

Prof. Herb Kaesz (USA), of the University of California at Los Angeles, former chairman of CNIC, past editor of *Inorganic Chemistry.*

Mr. Ole Nørager is Danish, but works at the European Chemicals Bureau, Toxicology and Chemical Substances, Institute for Health and Consumer Protection at the Ispra Joint Research Centre (Italy). Has been involved with chemicals databases such as EINECS (see below).

Mr. Kevin Thurlow (UK). Employed in the Chemical Nomenclature Advisory Service at the Laboratory of the Government Chemist. Nomenclature including INN and ISO pesticide names, analytical work, safety data sheets, customs legislation.

Dr. Andrey Yerin (Russia). Organic chemist, works with computer nomenclature rules at *ACD labs*, where they are now starting to consider inorganic compounds. Has worked for IUPAC in the former Commission on Nomenclature of Organic Chemistry (CNOC) and later Division VIII.

Mr. Jonathan Brecher (USA), at *Cambridge Soft* (known for products such as ChemDraw and ChemFinder). Strong interest in chemical communication. Is currently working towards the software required to convert structures to names.

Dr. Jeffrey Wilson (USA), Scientific Information Analysis Manager
at *Chemical Abstracts Systems* (*CAS*). Nomenclature of small molecules, general organic nomenclature.

Prof. Bryan Henry (Canada), of the University of Guelph. IUPAC vice-president. Laser chemistry. Canadian Chemical Society, national committee for IUPAC.

Dr. Alan Hutton (South Africa), of the University of Cape Town. Editor of *South African Journal of Chemistry*. Co-editor of the revised Red Book.

Dr. Alan McNaught (UK), of the Royal Society of Chemistry. Long-time involvement with (largely organic) IUPAC nomenclature, *e.g.* in CNOC. Has also been secretary of the former Interdivisional Committee on Nomenclature and Symbols (IDCNS) and is currently president of Division VIII.

Dr. Warren Powell (USA). Worked with Kurt Loening at *CAS*. Long-time involvement with IUPAC nomenclature in CNIC, CNOC and IDCNS and lately *e.g.* in nomenclature of fullerenes and as co-author of the new Blue Book. Has written two books on nomenclature. Currently secretary of Division VIII.

Prof. Richard Hartshorn (New Zealand), of the University of Canterbury. Teaches inorganic chemistry at large. Co-editor of the revised Red Book, involved with project on coordination numbers larger than 6.

Dr. Ture Damhus (Denmark), employed by *Novozymes A/S*. Earlier IUPAC involvement as member and secretary of CNIC. Co-editor of the revised Red Book.

Other potential participants that were not able to attend this meeting:

Prof. Ebbe Nordlander (Sweden), of the University of Lund.
Dr. David Lide (USA), Editor of *CRC Handbook of Chemistry and Physics*.

The attendees were asked to introduce themselves and explain about their possible interest in PINs and provide other relevant background.

Pertinent observations and comments included the following:

- In the public, there is often frustration that there is no unique IUPAC name for a given substance. This goes for example for people inquiring with the Royal Society of Chemistry in the UK and for customers using various kinds of computerized naming.
- Patent writing, chemicals catalogues and teaching would also benefit from unique names.
- Unambiguous names are important in shipping chemicals; the currently used so-called 'proper names' are not always easily interpreted.
- *Inorganic Syntheses* was mentioned as a relevant publication which is a good source of structures that need naming.
- Names and registry numbers assigned by *CAS* are useful in many contexts, but do not make IUPAC names superfluous. *CAS* is a commercial enterprise and could, in principle disappear again due to market conditions.
- The various layers of information involved in the assignment of an InChI (*IUPAC International Chemical Identifier*) should be considered. The *CAS* systematics for inorganic structures as presented in the Index Guide could maybe also be a useful starting point. Differences between IUPAC and *CAS* must be eventually documented.
- In real life, one often encounters mixtures or substances for which it may not be evident how to draw the structure on which to base the name (examples mentioned at the meeting: ascorbic acid, nitrogen dioxide, fulminic acid). It is often a question of whether to label the bottle or label specific structures. It may be dangerous to endeavour to select preferred structures.
- Preferred names may be given case by case in lists of names, or rules may be devised.
- Existing names should be used where possible. Extensive databases exist containing names (in some cases current IUPAC names) that were selected somehow and for which there are no resources to rename and republish.
- IUPAC should consider whether to promote organic PINs before inorganic PINs are available.

See also Appendix 1 for a communication from David Lide.

Based on the discussion, the following draft project objectives were agreed to:

Project Objectives

Provide rules for selecting a preferred name for any specified structure to complement the Blue Book PINs for organic compounds.

-Take preselected parent names (from the Blue Book) into consideration.
-Work closely with Chemical Abstracts Systems.
- Involve relevant databases (regulatory databases such as EINECS*), ELINCS**), ECICS***) dictionaries, maybe even vendors' catalogues; make contact to publishers)
- Collaborate with other bodies that potentially could have an interest in PINs [International Union of Crystallography, American Chemical Society (ACS), etc.]
- Coordinate with oncoming IUPAC project on organometallic nomenclature.

*) EINECS = European Inventory of Existing Commercial Substances
**) ELINCS = European List of Notified Chemical Substances
***) ECICS = European Customs Inventory of Chemical Substances

Comments

It will be necessary for the system to address several levels of compositional and structural information. In connection with the regulatory databases, it was mentioned that the European REACH project (REACH = Registration, Evaluation and Authorization of Chemicals) could conceivably be a "customer" for inorganic PINs.

Project group

It was recommended to strive for a two-tier project group with a small core, counting some 3-4 people, which would be responsible for main parts of the work, and a number of more loosely associated or corresponding members that could be consulted on specific issues.

Several attendees expressed willingness to either participate in the project group in one or the other tier or to establish contact to relevant persons in other bodies, *e.g.* ACS.

Future plans

[Subsequently, Ture Damhus unfortunately, for personal reasons, was not able to prepare for a meeting in Beijing to get the project started and has not accepted project leadership. The Division VIII Committee must consider in Beijing how to proceed. The following have in the meantime confirmed their willingness to be eventually members of the project group: Richard Hartshorn (core), Ebbe Nordlander (core or consultant), Kevin Thurlow (consultant), Alan Hutton (consultant).]

Ture Damhus

August 6, 2005

Appendix 1.

Communication from David Lide prior to the Budapest meeting.

Thanks very much for keeping me informed. My only suggestion is that you bear in mind the need for names for reaction intermediates and other transient molecular species. I recently spent much time finding names for transients that appear in tables of electron affinity, proton affinity, etc. A few examples:

> Radicals like AsH_2, PH_2, etc.
> Intermetallic compounds like AuPd, Au_2Pd, etc.
> Clusters like Al_3, Si_7, Sb_5, ...
> Simple compound that occur in two forms: NiO_2 can be O-Ni-O or Ni-O-O

I found that most authors who report measurements on things like this do not even try to name them. Obviously these are of lower priority than chemicals you can find in a bottle, but your approach should be applicable to them.

APPENDIX IV

Composition of the Advisory Subcommittee to the Division of Chemical Nomenclature and Structure Representation (IUPAC DIVISION VIII) (/13/05)

Dr Hidetsugu Abe (Toyohashi U of Technology, Japan)
Prof Steven M Bachrach (Trinity U San Antonio, USA; Editor, Internet Journal of Chemistry)
Dr Sinéad Boyce (Trinity College Dublin, Ireland)
Dr John Brennan (European Patent Office, Netherlands)
Dr Ursula Bünzli-Trepp (Helvetica Chimica Acta, Switzerland)
Dr Ilaria Campagnari (GSK, Italy)
Mr Jeffrey Carter (Cambridgesoft, USA)
Prof Neil G Connelly (Bristol, UK)
Dr Helen Cooke (GSK, USA)
Prof Franco Cozzi (Milan, Italy)
Prof Bernadette Donovan-Merkert (U of North Carolina, Charlotte, USA)
Prof Andreas Dress (Bielefeld, Germany)
Dr Geoff Fairhurst (BASF, Germany)
Prof Henri A Favre (Montreal, Canada)
Dr Piroska Fodor-Csányi (Budapest, Hungary)
Dr Patton M Giles (Chemical Abstracts, USA; ACS Nomenclature Committee)
Dr Jonathan M Goodman (Unilever Centre for Molecular Informatics, Cambridge, UK)
Dr Karl-Heinz Hellwich (Beilstein, Germany)
Prof Bernardo J Herold (Lisbon, Portugal)
Dr Alan T Hutton (Cape Town, South Africa)
Dr Wolf-Dietrich Ihlenfeldt (Computer Chem Center, Erlangen-Nurnberg, Germany)
Prof Aubrey D Jenkins (Sussex, UK)
Prof Alan R Katritzky (Florida Center for Heterocyclic Compounds, USA)
Prof Risto S Laitinen (Oulu, Finland)
Dr Graham F McCann (Royal Society of Chemistry, UK; Editor, J Materials Chem)
Prof Paulina Mata (Lisbon, Portugal)
Dr W Val Metanomski (Chemical Abstracts, USA)
Prof Ebbe Nordlander (Lund, Sweden)
Prof Vincent L Pecoraro (Michigan, USA; Assoc Editor, Inorg Chem)
Prof C Dale Poulter (Utah, USA; Editor, J Org Chem)
M Herve Schepers (European Commission Taxation and Customs Union, Bruxelles, Belgium)
Professor Alexander Senning (Technical University of Denmark)
Dr Ann Smith (Merck, USA)
Dr Steve Stein (NIST, USA)
Dr Keith Taylor (MDL, USA)
Dr Carlo Thilgen (ETH Zürich, Switzerland)
Dr Sarah Thomas (Royal Society of Chemistry, UK; Editor, ChemComm)
Mr Kevin Thurlow (LGC Nomenclature Advisory Service, UK)
Dr Bill Town (Kilmorie Consulting, UK)
Prof Jim Traynham (Baton Rouge, USA)
Dr Edward S Wilks (ex-Dupont, USA)
Dr Jeff Wilson (Chemical Abstracts, USA)
Dr Janusz L Wisniewski (MDL, Germany)
Dr Shen-Gang Yuan (Shanghai, China)

APPENDIX V

IUPAC Chemical Nomenclature and Structure Representation Division (VIII)

DIVISION RULES

1. The mission of the Chemical Nomenclature and Structure Representation Division is to maintain and develop standard systems for designating chemical structures, including both conventional nomenclature and computer-based systems. Terms of Reference are attached.

2. Under the Statutes, Bylaws, and policies of the Union, the Division is managed by its Division Committee. S10 and B4.1 and their subsections are particularly relevant. The Division Committee is responsible for initiating and managing scientific projects, symposia and other activities within its area of responsibility and for cooperating with other Divisions and Standing Committees in initiating and managing interdisciplinary projects, symposia and other activities.

3. In accord with B4.103, the composition of the Division Committee is as follows:

   (a) No more than 10 Titular Members (including all Officers as defined below)

   (b) No more than six Associate Members

   (c) No more than six National Representatives

4. (a) Titular Members of the Division Committee are nominated and elected for a term of four years by the electorate defined in B4.103 and Bureau decisions pursuant to B4.103. Candidates for titular membership are nominated by the Nominating Committee described below.

   (b) Associate Members may be elected by the Division Committee for a term of two years, subject to reelection for a second two-year term, as provided in B4.103.

   (c) National Representatives may be elected by the Division Committee on nomination by National Adhering Organizations for a term of two years, subject to reelection for a second two-year term, as provided in B4.103.

   (d) Interim appointments to fill vacancies on the Division Committee occurring between meetings may be made by the Division President, after consultation with the other Division Officers, for a term ending at the end of the year in which the next General Assembly is held. Interim appointments are subject to approval by the Bureau or Executive Committee.

5. Candidates for Titular Member of the Division Committee are named by a Nominating Committee, prescribed by IUPAC policy and procedures defined by the Bureau, as follows:

(a) The nominating committee consists of five members [subject to an exception by the Bureau], with no more than two members from the existing Division Committee and the other three chosen from outside IUPAC on the basis of the breadth of their expertise. The Division President will not be a member of the Nominating Committee.

(b) The Nominating Committee is appointed by the Division President with the concurrence of the IUPAC Executive Committee.

(c) Categories of vacancies may be established by the Division Committee if desired to ensure diversity in subject matter, geographic distribution, or other characteristics. More than one nominee for each vacancy is desirable but not required.

6. Elections shall be conducted by e-mail under procedures defined by the IUPAC Secretariat.

7. The Officers of the Division are as follows:

(a) The President is the administrative head of the Division, presides at meetings of the Division Committee, and is an *ex officio* a member of all bodies of the Division. The President serves as a member of the Bureau and is the principal representative of the Division within and outside the Union.

(b) The Vice President (President-elect) acts for the President in his absence and assists the President as requested. He shall assume the office of Division President in the event of the President being unable to perform the functions of that office, without prejudice to the forthcoming period of office as President.

(c) The Secretary assists the President in carrying out the business of the Division and maintains the records of the Division.

(d) The immediate Past President assists the President as requested.

8. With the advice of the President of the Union, Officers of the Division are elected by the Division Committee, subject to final approval by the Council. The Officers together form an Executive Committee to act for the Division Committee between meetings. Subject to limitations in B4.103, the terms of office are as follows:

(a) The President, President-elect and Past President each serve a term of two [four] years, not subject to reelection.

(b) The Secretary serves a term of four years and is eligible for reelection to a second term of four years.

9. (a) The Division Committee may establish and the Division President may appoint subsidiary bodies, such as subcommittees, working parties and advisory groups, which will all have the status of Division subcommittees, as described in S10.6. The terms of reference or

charge to each group, as well as its lifetime, shall be established by the Division Committee. Task groups will be formed to carry out specific projects under general IUPAC policies for the conduct of projects.

(b) The Division Committee may propose to the Bureau the establishment of Commissions, with terms of reference and lifetimes, under the provisions of B4.301.

(c) The Division Committee and Division President will exercise responsibility and oversight over all bodies created under parts (a) and (b).

10. These Rules may be amended by the Division Committee, subject to approval by the Council.

APPENDIX VI

Nomenclature World Wide Web Database – Statistics

Statistics based on log of IP addresses used each day. Total usage to date about 3930000. Data on 190 countries recorded so far. Summary data for 1996-2004 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	2005
Total usage	296	650	1476	2786	5515	9813	15360	19105	20392	24591
Search Facility	-	-	-	204	1663	4169	8355	11308	12192	15350
Bibliographic Data	-	61	142	235	325	470	598	655	706	828
Map of Usage	-	7	8	29	37	58	83	78	107	138
IUPAC Nomenclature										
Class Names Glossary	138	157	430	693	1039	1504	2178	2492	2836	3139
Atomic Weight	23	48	95	144	310	651	964	1431	1525	1798
Physical Org Chem Glossary	29	36	136	343	751	1089	1796	1934	1782	1756
Periodic Table	-	-	-	17	155	291	475	870	782	920
Stereochemical Glossary	-	32	85	135	231	392	602	694	778	864
Section F (Natural Products)	-	-	-	14	121	321	450	505	583	819
Medicinal Chemistry Glossary	-	-	56	87	150	316	532	601	636	713
Bioinorganic Glossary	-	-	61	108	201	391	633	570	523	640
Fused Ring	-	-	64	73	110	198	241	275	299	330
Numerical Term	-	18	27	35	54	99	150	189	238	308
Ions and Radicals	-	-	-	-	72	150	196	226	245	278
Regular Organic Polymer	-	-	-	-	-	-	-	-	141	231
Phanes	-	-	31	42	56	80	95	135	181	213
Gold Book	-	-	-	-	80	127	155	162	186	212
Fullerenes	-	-	-	-	-	-	69	124	162	202
Hantzsch Widman	12	14	31	46	56	89	116	125	154	187
Spiro	-		-	26	47	90	114	115	137	152
von Baeyer	-	-	-	29	61	106	130	118	133	145
Delta Convention	8	9	19	30	54	82	110	106	121	140
Element Name > 100	-	-	-	20	45	78	87	93	147	137
Section H (Isotopic Label)	-	-	26	34	46	73	90	93	112	121
Lambda Convention	6	8	17	28	40	60	76	74	85	98
Phane II	-	-	-	-	-	-	-	59	68	87
Guide Errata	-	-	-	20	21	25	32	47	53	60
Fullerene II	-	-	-	-	-	-	-	-	-	-

	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005
IUPAC/IUBMB Nomenclature										
Amino Acids & Peptides	31	62	135	186	359	670	1072	1366	1594	1936
Carbohydrates	46	72	144	237	453	835	1156	1444	1266	1307
Steroids	12	21	87	93	396	811	1213	1460	835	620
Vitamin D	-	-	-	-	47	69	125	209	385	395
Nucleic Acid Abbreviations	-	-	-	45	77	136	202	241	256	303
Tetrapyrroles	-	-	-	-	-	124	221	227	240	299
Lipids	-	-	-	29	70	132	198	232	252	297
Vitamin B-6	-	-	-	34	95	155	267	466	306	265
Folic acid	-	-	-	60	58	210	208	304	284	248
Tocopherol	-	-	21	33	48	80	150	274	232	245
Glycoproteins	-	-	20	32	71	134	172	187	185	224
Glycolipids	-	-	15	35	65	91	137	171	213	217
Polypeptide Conformation	-	8	14	34	61	111	173	191	182	200
Lignans and Neolignans	-	-	-	-	-	71	123	137	170	208
Carotenoids	-	-	-	-	46	84	128	148	167	199
Cyclitols	-	-	21	51	72	113	174	178	177	196
Polysaccharide Conformation	-	8	14	26	49	82	134	153	155	156
Quinones with Isoprenoid Chain	-	-	-	-	-	47	90	105	116	150
Polynucleotide Conformation	-	7	15	27	44	68	92	103	124	148
Retinoids	-	-	-	-	35	71	99	126	140	146
Vitamin B-12	-	-	-	49	69	146	266	315	227	144
Biochemical Phosphorus	-	-	-	-	62	103	151	147	133	143
Prenols	-	-	-	19	33	55	77	84	108	123
Polymerised Peptides	-	-	-	-	34	56	91	97	109	112
Both Committees										
Committees' Homepage	18	38	65	123	268	423	653	801	1015	1267
Newsletter	-	-	25	59	145	304	456	446	490	613
IUBMB Nomenclature										
Enzymes	16	54	124	320	1086	2088	3560	4260	5459	8364
EC 1	-	-	-	35	241	487	922	1091	1497	2503
EC 2	-	-	-	-	180	438	769	900	1242	2086
EC 3	-	-	-	-	165	427	947	1054	1496	2333
EC 3.4 (50 file)	16	54	>82	200	285	281	184	114	110	137
EC 3.4 (single)	-	-	-	-	-	134	343	397	589	890
EC 3.4 (total)	-	-	-	-	-	336	484	472	654	975
EC 4	-	-	-	-	90	223	410	423	635	1061
EC 5	-	-	-	-	64	164	294	322	441	649
EC 6	-	-	-	-	46	138	239	261	374	590

	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005
reaction	-	-	-	-	48	119	381	650	1089	2073
newenz	-	-	-	-	53	60	75	71	86	89
Enzyme Supplement 5	-	-	42	66	79	53	37	29	33	31
Enzyme Kinetics	-	-	16	61	152	249	365	441	547	652
Incomplete Nuc. Acid Sequence	-	9	20	31	50	75	103	137	205	307
Membrane Transport Proteins	-	-	-	-	-	-	93	157	188	264
Biochemical Thermodynamics	-	-	22	40	66	107	132	148	170	213
Electron Transport Proteins	-	-	-	-	58	107	163	165	168	204
Isoenzymes	-	-	14	28	68	106	124	123	135	181
Peptide Hormones	-	-	-	-	32	51	80	101	115	135
myo-inositol	-	-	11	23	43	74	125	125	113	128
Branched Chain Nucleic Acids	-	3	6	10	40	63	115	107	89	108
Translation Factors	-	-	-	-	11	18	34	37	42	49
Multienzymes	-	-	10	13	18	25	37	36	43	48

GPM
11 April 2005

APPENDIX VII

Translations of IUPAC Recommendations and Technical Reports into German

Since 2002 the journal *Angewandte Chemie* (*Angew. Chem.*) has been publishing translations of IUPAC Recommendations and Technical Reports into German.

A total of 8 translations were published in 2002.
5 translations appeared each in 2003 and 2004.
By the end of 2005 four further translations will have been published.
The translation published most recently is "Nomenclature of Fullerenes C_{60}-I_h und C_{70}-$D_{5h(6)}$" which appeared in issue 31 of *Angew. Chem.* 2005.
The next translation to be published is the Natural Products Nomenclature (Revised Section F), which includes the corrections and modifications published in *Pure Appl. Chem.* in 2004.

The editior of the German translation of "*A Guide to IUPAC Nomenclature of Organic Compounds, Recommendations 1993*", Ms. Gerlinde Kruse, died on July 30, 2005.

Deutsche Übersetzungen von IUPAC-Veröffentlichungen

Stefan Bräse,* Burkard Neuß
Glossar von Begriffen der Kombinatorischen Chemie
Angew. Chem. **2002**, *114, Nr. 5*, 893 – 906
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