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

Torino, Italy, August 4-5, 2007

Members present: Mr Jonathan Brecher, Dr Ture Damhus**,** Prof Richard Hartshorn, Dr Stephen Heller, Dr Karl-Heinz Hellwich, Prof Alan T. Hutton, Prof Richard Jones, Dr Jaroslav Kahovec, Prof G Jeffery Leigh, Dr Alan D McNaught (Past President), Dr Gerard Moss (President), Prof József Nyitrai, Dr Warren Powell (Secretary), Dr Jeffrey Wilson, Dr Andrey Yerin

National Representative Present: Prof Hiroshi Ogino (Japan, Associate Member, ICTNS);

Observers: Dr Kirill Degtyarenko, in part (Task Group, Graphical Representation Standards); Ms Danièle Gibney (Young Observer, Technical Editor, RSC Publishing, UK); Prof Michael Scott (Young Observer, University of Florida, USA)

Members Absent: Prof Franco Cozzi

Others: Prof Tatsuki Kitayama, in part (Project Leader, Nomenclature of Chemically Modified Polymers)

The seventh meeting of the Division Committee of the IUPAC Division of Chemical Nomenclature and Structure Representation held during the 44th General Assembly Meeting at the University of Torino and the Polytecnico of Torino in the Lingotto in Torino, Italy, was convened by President Moss at 9:00 on August 4, 2007.

1.0 Introductory Remarks. President Moss welcomed the members to this meeting and offered a special welcome to the young observers Ms Danièle Gibney, a Technical Editor at RSC Publishing, UK and Prof Michael Scott from the University of Florida, USA. Each of the attendees introduced themselves and provided some background information. Housekeeping details regarding breaks and lunch were announced.

2.0 Apologies for absence. None were received.

3.0 Approval of Agenda. The circulated agenda was approved with the following changes;

(1) Membership. Announcement of the results of the titular membership, the election of Vice-President and Secretary would be inserted into the agenda following the matters arising from the minutes of the Prague minutes.

(2) Topics related to the new Red Book would be discussed as item 11.0.

(3) C-SMILES as an alternative to InChI will be considered at a convenient time in the agenda.

(4) Dr. Mark Cesa, Chairman of the Committee on Chemistry and Industry (COCI) will speak to the Division Committee at 11:00 on August 4.

(5) Prof Peter Mahaffy and Prof Eva Åkesson, Chairman and Secretary, respectively of the Committee on Chemical Education will speak to the Division Committee at 14:45 on August 5.

4.0 Minutes of the Prague meeting. A number of typographical errors were noted and will be transferred to the file on the IUPAC website. Other corrections made were as follows:

(1) Minute 13.2.1. The first sentence of the second paragraph was changed to read as follows: 'The IUPAC website appears to be for use by IUPAC members and not for the general public.'

(2) Minute 14.4. This minute was changed to read as follows: 'Recommendations better reflect the status of IUPAC rules and are without any power of enforcement.'

5.0 Matters arising from the Prague minutes

(1) A manuscript "Improving the Quality of Published Chemical Names with Nomenclature Software" by Gernot Eller had been sent to Dr Moss for evaluation as a publication for *Pure and Applied Chemistry* (see minute 14.2, Prague minutes). Following discussion and comments from Division Members, Dr Moss replied on behalf of the Division. The correspondence is given in Appendix I.

(2) In Prague, Dr Hellwich asked for advice on how to deal with requests for IUPAC names that he receives (see minute 14.3, Prague minutes). In answer, it was noted that IUPAC (Division VIII) has no obligation to respond. For the future, the Secretariat should be asked how to deal with questions directed to Division VIII on the IUPAC website. Dr Moss will follow-up on this question with the Secretariat.

6.0 Titular Membership, Vice-President, and Secretary.

6.1 Following the procedure of Division VIII for the election of Titular Members, the following were elected to Titular Membership for 2008-2011

Mr Jonathan Brecher
Prof Alan T. Hutton
Prof G. Jeffery Leigh
Prof Philip Hodge
Dr Jeffrey Wilson
Dr Kirill Degtyarenko

Prof Leigh raised a point regarding the election procedure. The issue was that a person should be approached about being a nominee for Titular Membership and should be informed if elected. This issue is supposed to be a responsibility of the Nominating Committee. Paul LeClair should be approached about this. The existing rules for Division elections should be put on the agenda for discussion at next year's meeting.

6.2 Dr Karl-Heinz Hellwich and Prof Richard Hartshorn had been nominated as candidates for the office of Vice-President. Prof Hartshorn was elected.

6.3 In Prague, Dr Powell had announced that he would not continue beyond 2007 as Secretary of the Division. As the only candidate for the office of Secretary, Dr Ture Damhus was elected.

7.0 The IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN). The Joint Commission met in Chevy Chase, MD on May 5-6, 2007 with the NC-IUBMB (Nomenclature Committee of the International Union of Biochemistry and Molecular Biology). The minutes of the meeting are given as Appendix II.

7.1 The meeting dealt mainly with topics related to enzymes. It was suggested that there be a special category of membership to deal specifically with the various aspects related to the enzyme database, such as interaction with other databases that have some relationship with the enzyme database, and cross correlation with CAS. CAS registry numbers are given in the enzyme database where available.

7.2 There is an ongoing revision of the 1996 publication on carbohydrate document, headed by Derek Horton. Comments on the 1986 document should be sent to him. There also is a need for a carbohydrate nomenclature document more suited to the biochemical community rather that synthetic chemist. Dr Moss noted that this revision will address polysaccharides and conjugates more extensively than the old publication.

7.3 Dr McNaught and Dr Moss are involved in a project to compile a list of molecules of importance to biochemistry that have not been covered by other nomenclature documents. Its aim is to provide structure and numbering information for molecules such as thiamine diphosphate, riboflavin and coenzyme A that are very common but for which it is difficult to find such information.

7.4 The recommendation of a year ago to change the format of locants for nitrogen substituents of amino acids from N^6- to 6-*N* was not accepted by IUPAC and will not be used in biochemical documents.

7.5 A document on nomenclature of phosphorus compounds of biochemical importance will be ready soon to forward to IUPAC for review.

8.0 Publications and Presentations

8.1 "Graphical Representation of Stereochemical Configuration, (IUPAC Recommendations 2006)", Prepared for Publication by Jonathan Brecher, *Pure Appl. Chem*., **78**(10), 1897–1970 (2006).

8.2 "Tools of the Trade: The Red Book – Nomenclature of Inorganic Chemistry IUPAC Recommendations 2005", Richard Hartshorn, *Chem. Int*., in press.

8.3 The German translation of Phane Nomenclature, Part II , *Pure Appl. Chem*. **74**, 809–834 (2002) that was noted in Prague minute 12.4.1 for planned publication late in 2006 has appeared: "Phannomenklatur Teil II: Änderung des Hydrierungsgrades und Substitutionsderivate von Phanstammverbindungen", *Angew. Chem*. **2006**, 118 (35), 6023–6033 (2006) (Karl-Heinz Hellwich, Kerstin Ibrom).

8.4 "Stereochemistry – Workbook (English edition), Karl-Heinz Hellwich, Carsten Siebert, Springer, 2006.

8.5 "Systematic Nomenclature of Organic, Organometallic, and Coordination Chemistry: Chemical Abstracts Guidelines with IUPAC Recommendations and Many Trivial Names", Ursula Bünzli-Trepp, EPFL Press.

8.7 CAS has made changes in its index nomenclature effective with the beginning of the 16th Collective Period (2007). A document outlining these changes can be found at:

http://www.cas.org/ASSETS/ADB8C3A6495849638F4897BFE7B893B3/caindexname.pdf

9.0 Division VIII projects

9.1 The IUPAC International Chemical Idenifier (InChI) (2007-019-1-800). Dr McNaught provided a report on the InChI project. His full report is given as Appendix III.

9.1.1 Dr Heller continues to give talks on InChI. The list of his meetings and presentations are in Dr McNaught's report. Dr Heller's slides are available at:

http://www.hellers.com/steve/pub-talks

9.1.2 In his capacity as a representative of Division VIII on the InChI project group, Dr McNaught received a paper "C-SMILES: A Language to Specify Molecules", by J. Hinze, A Bruder, and T. Tusing from the University of Bielefeld. It was circulated to members of the Division Committee for comment. Many comments were received, mostly opposed. Dr McNaught will collate the comments and reply to Prof Hinze.

9.1.3 The project group has been asked to prepare a comprehensive paper for publication. This is underway.

9.1.4 Future efforts will focus on creating a critical mass if InChI data in the primary journal literature on the web.

9.2 Preferred names in the Nomenclature of Organic Compounds (2001-043-1-800). Dr Powell reported that the majority of the time during the past year was spent in attempting to implement the changes in Chapters 1, 4 and 5 that were agreed last year in Prague (see minute 8.2 in the Prague minutes) and in editing P-60-64 in Chapter 6. At this time, only Chapters 2, 3, 9 and 10 can be considered to be complete. Prof Favre and Dr Hellwich are collaborating on Chapter 9 and Prof Favre and Dr McNaught on Chapter 10.

9.2.1 A working group consisting of Prof Favre, Dr Powell, and Dr McNaught met in Turin on August 2 to consider the revisions of Chapters 1, 4, and 5, as well as Chapters 7 and 8, which were not comprehensively reviewed at the Boston meeting in April, 2005. Prof Favre raised several questions regarding the revisions for Chapters 1, 4, and 5 which were discussed thoroughly and, as a result, considerable revision to these Chapters will be necessary. The project group recommended that Chapter 5 dealing with criteria for selecting PINs be moved to follow Chapters 6, 7, 8 and perhaps 9 in order to include selection criteria now given in the applications chapters 6,7,8 and 9. This proposal was REJECTED by the Division Committee.

9.2.2 Prof Hartshorn introduced the concept of multiple levels of PINs, particularly with regard to knowledge of only empirical formulas and only partial stereochemistry. The first point is important to the development of inorganic PINs; it is more important to inorganic compounds than to organic compounds. The second point would be the same as for organic compounds. Different InChIs would be produced depending on the degree of stereochemical knowledge given by the input formula.

9.2.3 Prof Hartshorn asked that the vertical line of demarcation between Groups 12 and 13 for determining the responsibility for establishing IUPAC PINs set up by the alignment task group be reconsidered and reproduced in the current

draft of the revised Blue Book (see minute 9.11). The task group for inorganic PINs recommends a stepped line similar to the earlier stepped line marking the separation of the metals from the nonmetals and/or metalloids. It was noted that such a line would only refer to the responsibility for determining a PIN, and not necessarily the type of nomenclature to be used.

9.2.4 Dr Damhus raised the question of preselected names for oxy acids with no carbon and the 'inorganic' carbon acids, comparing the names trithiocarbonate and trisulfidocarbonate. He asked whether carbonic acid and its replacement analogs with no other carbon atoms should be an exception to the carbon requirement for treatment by the new Blue Book. No conclusion was reached.

9.2.5 The use of the acronym PIN for substituent prefixes was questioned. The acronym PIP for preferred IUPAC prefix was accepted. Dr Powell noted that it really isn't the substituent prefix itself that is preferred; it is the name of the prefix that is preferred, which would lead to the acronym PIPN.

9.2.6 For planning purposes, the publisher, RSC, had requested information about a date that they might expect a manuscript to be delivered to them. The date that was given for a complete manuscript from the authors was April, 2008. This date does not include any time for any review process. However, as a result of the meeting of the project group here in Turin, Dr Powell expressed reservations as to whether this could be considered an attainable date.

9.2.6 Since the revised Blue Book has undergone considerable changes since the September, 2004 manuscript was reviewed, the current manuscript will need some kind of review. After some discussion, it seemed to be agreed that as each chapter is completed by the authors it be distributed to the Division Committee via the Division VIII Webboard for review as rapidly as possible.

9.3 Nomenclature for Rotaxanes (2002-007-1-899) Following the large number of comments and suggestions made during the public and expert review of this manuscript, the recommendations have been significantly changed. In addition to several terminology and many text changes, the main changes were announced by Dr Yerin as follows:

9.3.1 The title has been changed to "Nomenclature for Rotaxanes and Pseudorotaxanes"

9.3.2 The definitions of rotaxanes and pseudortaxanes are modified to maintain the principal difference between these two classes of threaded molecules.

9.3.3 The descriptors *A* and *C* proposed initially to define stereoisomers were changed to *M* and *P* for unity with descriptors currently proposed for describing complex stereogenic units, i.e., axes, planes, and helix. Dr Hellwich raised a serious objections to this change, namely that *M* and *P* are used to indicate the helicity of a system by describing the direction of a dihedral angle between a part of the structure nearer to the observer and another part more distant from the observer. However, the rotaxanes for which these descriptors were proposed do not exhibit helical chirality. Since a ring is not a helix, and a dihedral angle cannot be defined from one direction, the stereodescriptors *M* and *P* are inappropriate. The descriptors *C* and *A* do describe a direction and are fully appropriate for the structures

under discussion. However, there might be a fixed orientation of two rings with respect to each other in addition to the orientation of the rings with respect to the direction of the linear component which then would, in fact, exhibit helical chirality. Hence, the descriptors *M* and *P* might be needed in addition to *C* and *A*. Dr Yerin will reinstate the use of the descriptors *C* and *A* in the document.

9.3.4 The descriptors *ab* and *ba* to define rotaxane isomers with unsymmetrical rings with different sides were changed into the traditional descriptors *syn* and *anti* that clearly define a spatial relationship of fragments.

9.3.5 The enclosing marks for the names of the rotaxane components and the entire rotaxane name are defined as fixed; brackets for component names and braces for the entire name. This makes the procedure simpler. Systematic names are often quite complex and the choice of enclosing marks according to the accepted nesting order can be a difficult procedure.

9.3.6 The updated document (Version H) can be considered as final. It was submitted to ICTNS and distributed to the project group members in June, 2007.

9.4 Extension of IUPAC Rules for Stereodescriptors to Coordination numbers 7-12 (2003-025-1). The final report of the project "Representation of Coordination Polyhedra and the Extension of Current Methodology" (see also minute 8.4, Prague minutes) was submitted as a Technical Report. It is following the normal review process for Technical Reports. The conclusions of this project were that the method adopted for coordination numbers up through 6 cannot be pushed very far. The structures are too far from ideal geometries. Some geometries with coordination number 8 can be done and a very few geometries with coordination number 9. Essentially no geometries with coordination numbers 10-12 can be described by this method.

9.5 Macromolecular Projects (Joint with Division IV)

9.5.1 Purple Book, 2nd Ed. (2002-048-1-400) Prof R. Jones, Chairman of the Division IV Subcommittee on Polymer Terminology, presented a report on the status of the project to produce a new edition of the Purple Book "The Compendium of Macromolecular Terminology and Nomenclature". This project essentially stalled in 2005. In Prague, the decision was made to basically start over. All terminology chapters were reviewed for errors and consistency. All nomenclature chapters were carefully reviewed. As a result the complete Revised Purple Book is here in Turin and should appear in print by the first of the year or shortly thereafter.

9.5.2 Source-Based Nomenclature of Single-Strand Organic Polymers (2003-042-1-800). Prof Kitayama, Task Group Chairman, discussed the status of this project and distributed an edited draft and some notes and proposals to be discussed at the meeting of Division IV next week. Both systematic names according to the Blue Book and 'names retained for use in polymer names' will be included and related by footnotes. This edited draft will be discussed here in Turin and when accepted by Division IV will be sent electronically to Division VIII for distribution on the Division VIII Webboard.

9.5.3 Nomenclature for Chemically Modified Polymer Molecules (1999-051-1-800) (Extended Project 2006-006-1-400; formerly Project 33/99). Prof Kitayama,

Task Group Chairman, noted that the name for the document from this Task Group is now "Nomenclature and Graphic Representation for Chemically Modified Polymers". The term '*mod*' is the indicator for a modified polymer and can have two different meanings. The current draft will be discussed in Division IV here in Turin and after correction and acceptance by Division IV will be sent electronically to Division VIII for distribution to Division VIII members by means of the Webboard.

9.5.4 Nomenclature for (Macromolecular) Rotaxanes. Dr. Yerin reported that this project began in 2000 as a project on the "Nomenclature of Rotaxanes, Catenanes, and Macromolecular Rotaxanes" (see *Chem. Int*., May, 2002) which changed almost immediately to the "Nomenclature of Macromolecular Rotaxanes" (2000-037-1-800: previously 2000-037-1-400) and then to just "Nomenclature of Rotaxanes" (2002-007-1-800) because it would be logical to develop general recommendations on rotaxanes and then make recommendations on macromolecular rotaxanes, a specific kind of rotaxane. Since the project on the "Nomenclature of Rotaxanes" can be considered as finished (see minute 9.3 above), a new joint project between Division IV and Division VIII, "Nomenclature for Rotaxane Polymers" (2007-009-1-800) was initiated and approved. The first meeting of this task group led by Prof. Jiri Vohlidal of Division IV is scheduled for later in this Turin General Assembly meeting. The significant part of the work done for the project "Nomenclature for Macromolecular Rotaxanes (2000-037-1-800) was used as the basis for the project "Nomenclature for Rotaxanes". Then, the specific parts of the macromolecular rotaxanes report dealing with macromolecules, with changes made to follow the general recommendations for rotaxanes, will be used as the first draft of the new document "Nomenclature for Macromolecular Rotaxanes (2000-037-1-800).

9.5.5 Terminology and Structure-Based Nomenclature of Dendritic and Hyperbranched Polymers (2000-081-1-800). Dr Kahovec reported that terminology problems are still evident which prevent this document from proceeding ahead in a normal manner. Hence, the document has been divided into two parts, one for dendritic polymers and one for hyperbranched polymers. The two documents are ready to be submitted for Division VIII review. Dr Kahovec will send them to Dr McNaught to be placed on the Division VIII Webboard. It was suggested that 'Organic' be added to the titles.

9.5.6 Terminology and Nomenclature of Macromolecules with Cyclic Structures (2001-082-1-800; extension 2004-046-1-800). Dr Hellwich reported that, following the Meetings in Prague, he and Prof Mormann checked all of the references, updating those to the Gold Book and the Red Book, and cross-references, made the necessary formal corrections, and submitted the manuscript to the Secretariat for the ICTNS and public reviews. On May 30 the results of the review were transmitted to Prof Mormann. There were 9 reviewers only 4 of which submitted comments, two of which were only typographical in nature. One reviewer suggested that a major part of the document should be removed, the part that had been explicitly included by the extension of the project as a result of a literature search, because such compounds would never be prepared This reviewer clearly failed to notice the

explicit statement in the paper that these examples were taken from the cited references. Also, such an argument should be completely discounted since a large number of examples in all IUPAC documents are compounds that have never been, or even maybe will never be, prepared and are included to emphasize the scope of the recommendations.

ICTNS has recommended that publication of this report be delayed until after the appearance of the revised Blue Book. However, the Division VIII Committee agreed that publication should not be delayed. Further, the Division VIII Committee recommended that since italic type in chemical names carries special meanings, italicization of terms mentioned in the main text be limited to terms mentioned in the Glossary.

This report will be given to the Division IV Subcommittee on Polymer Terminology for consideration at its meeting latter in the Turin GA meeting.

9.6. Cyclic Peptides (2004-024-1-800. Dr. Moss reported that there was no change in the status of the project since last year (see minute 8.6 in the Prague minutes.

9.7 Graphical Representation Standards for Chemical Structure Diagrams (2003-045-1-800) Mr. Brecher noted the publication of the report "Graphical Representation of Stereochemical Configuration, (IUPAC Recommendations 2006)" in *Pure Appl. Chem*., **78**(10), 1897-1970 (2006) (see minute 8.1, above). A near final draft of the next document to be considered by the project group which will cover virtually everything else for chemical structure diagrams (not including polymers), for example, orientation, bond widths, charges, was discussed at a meeting of the project group here in Turin. A final document should be ready to be submitted for publication shortly after this meeting. Other topics to be considered by the project group might include macromolecular structures such as polymers.

The question of dissemination of these recommendations was discussed at some length and included the following:

(1) distribution to schools and the like should be discussed with the Committee on Chemical Education when they meet with us later.

(2) Combine with the recommendations on stereochemical configuration and publish as a book.

(3) Newsletter-type publications in journals like *Chemistry*, *Chem. World,* and *Chem. Eng. News*.

(4) Include notices in instructions to authors, especially PAC and CI.

ICTNS should ensure that they be followed by authors in recommendations and technical reports. The new edition of *Principles of Chemical Nomenclature, A Guide to IUPAC Recommendations* should promote these recommendations.

9.8 Nomenclature of Phosphorus Containing Compounds of Biochemical Importance (2006-019-1-800).

A draft document produced for the JCBN meeting in Chevy Chase, MD, is a reorganization of the 1976 publication. It contains an expansion of recommendations for naming nucleotides, especially with regard to stereochemistry around phosphorus atoms. The term 'all-ambo' was proposed for the configuration of phosphorus atoms in polynucleotides with chiral thiophosphate groups. This document will be put on the Division VIII Webboard before going to ICTNS.

9.9 Comparison of procedures for naming hydro derivatives of fused ring systems.

Dr Powell reported that there was no change in the status of this project since last year (see minute 8.9 in the Prague meeting minutes)

9.10 The 2nd Edition of *Principles of Chemical Nomenclature, A Guide to IUPAC Recommendations* (2006-029-1-800).

Prof Leigh reported on the meeting of the Project Task group held on Aug 3, here in Turin. The program of work and those who are to do the work have all been agreed. An outline of the plan for the pattern of work and the amendments agreed during the meeting are given in Appendix IV. The section on biochemical nomenclature is to be expanded from the first edition. For the project group meeting, material received from Prof Favre and Prof Hess on organic and macromolecular nomenclature, respectively, was discussed. The general feeling was that this material was too detailed. A flow diagram will be prepared, if possible. Since no new nomenclature is to be included, reviews of the final manuscript should be minimal although it was pointed out that some form of ICTNS review would be valuable and could not be obviated. Details for such a review will be determined next year after wider discussions.

A suggestion to use colored pages to indicate different sections was offered.

The next meeting of the Project Task Group will be in August, 2008. A final meeting of all writers and reviewers is scheduled for late 2008 or early 2009 when the edited manuscripts will be reviewed by the various contributors. As yet, there are no plans for choice of publisher, publicity, or advertisement.

9.11 Preferred names for inorganic compounds (2006-038-1-800)

Prof Hartshorn reported on the meeting of the Project Task Group on Inorganic PINs held here in Turin on August 1-2. Of specific interest to the organic PINs project were the following:

(1) Moving the line of demarcation between the responsibility for assignment of PINs from the vertical line between Groups 12 and 13 to a stepped line similar to the 'old' line separating the nonmetals/semimetals from metals/semimetals. A proposal for discussion is given in Appendix V.

(2) The responsibility for PINs for compounds in groups 13-17 that do not contain carbon, such as thiosulfuric acid. And, a related question about responsibility for carbonic acid, itself, and some of its derivatives.

(3) Names for delocalized ions to be used as ligand names.

These topics probably should be discussed jointly by the inorganic PINs task group and the organic PINs task group.

9.12 Interdivisional Projects

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

This project is essentially stalled. The project leader became ill and had to drop his responsibilities for it.

9.12.2 Recommendations for nomenclature and databases for biochemical thermodynamics (2006-023-3-100).

This is mainly a Division I project but with JCBN representation on the project group. It was not discussed at the JCBN meeting in Chevy Chase.

No new information was presented on this project.

10. Future Projects

10.1 Preferred Structure-based Names for Macromolecules.

Division VIII needs to develop this project with significant contribution from Division IV. Dr Hellwich will attend the Division IV Subcommittee on Polymer Terminology.

10.2 Metallacycles.

Prof Hutton has contacted a number of people to assess their interest in such a project. Prof Kaesz will participate as an observer. Prof Yamamoto and Dr. Casey declined. Edwin Constable and Albert Salzer will participate

Dr. Wilson should be involved as a contact person for CAS involvement.

The project title probably should be broadened to something like 'Metallacycles and Related Compounds'

10.3 Boron Nomenclature.

Dr McNaught has spent a lot of time, primarily through contacts with the organizing committees for Boron Conferences, looking for someone to lead a project on boron nomenclature, without any success. The subject may have to be broken down into smaller bits, such as organoboron, simple boron hydrides, and boron clusters. Even before the new Red Book was published, there were publications by Powell, Sloan, Casey, and Evans to evaluate. And now there is fullerene numbering that might overlap with boron numberings to consider.

10.4 Other Potential Projects.

10.4.1 Division II would like to see a project on cluster nomenclature, but because of funding it would not be a joint project, but a Division VIII project. Prof Leigh presumably will be involved.

10.4.2 PINs for substances in the bottle.

10.4.3 Develop a flow chart for nomenclature. Mr Godly has published such a flow chart based on what would become the 1979 edition of the organic nomenclature recommendations: E. W. Godly, *Naming Organic Compounds, a systematic instruction manual*, Ellis Horwood, Chichester, UK, 1989. The 2005 edition of the *Nomenclature of Inorganic Chemistry* has a flow chart for inorganic compounds (see Figure IR-1.1, page 9).

10.4.4 Develop InChI for the molecular formula level.

10.4.5 Calixarenes. This was part of a very broad project along with rotaxanes and catenanes.

10.4.6 Numbering of total molecules for NMR and crystallography. This should probably be a joint project with Division I.

10.4.7 Graphical representation for polymer structures and reactions.

10.4.8 Configuration and stereodescriptors of polymers. Contributors with expertise in polymer stereochemistry are needed.

10.4.9 Revisit inorganic polymers

11. Associate Members, National Representatives, and Advisory Subcommittee

11.1 The following Titular Members who were retiring or had reached the end of their terms accepted appointments as Associate Members

Dr Warren Powell

Dr. Andrey Yerin

Prof Józef Nyitrai

Dr Jaroslav Kahovec

Prof Dr Sandy Lawson and Prof Ebbe Nordlander were contacted and agreed to become Associate Members.

11.2 National Representatives

Prof Farzana Ansari (Pakistan), Prof Ivan Dukov (Bulgaria), MDA Hashem (Bangladesh), Prof Lauri Lajunen (Finland), Prof Haroshi Ogino (Japan), Prof Jan Reedijk (Netherlands), Prof Youngkyu (Korea) were appointed as National Representatives.

11.3 Advisory Subcommittee.

Suggestions for additions to the Advisory Subcommittee included:Dr Michael Scott (University of Florida), Ms Danièle Gibney (RSC Publishing), Prof Eva Hey-Hawkins (member of the "Extension of IUPAC rules for stereodescriptors to include coordination numbers 7-12 project team), Prof Amelia Rauter (Lisbon, Division III Representative on ICTNS), Roger Sayle (OpenEye's Vice-President of Bioinformatics), Dr Gernot Eller (Austria), Gregory J Wilson (Australia).

The Portugese and Spanish translators of IUPAC documents could also be added to the Advisory Subcommittee.

12. New Red Book. Only a few comments have been received about the revised edition of the *Nomenclature of Inorganic Chemistry, IUPAC Recommendations 2005*, published by RSC Publishing, mostly dealing with the omission of alternative names for the elements. A member of Division II wants the name wolfram to be listed as well as the name tungsten. Dr Moss noted that no editions of the Red Book since 1970 have recommended the use of the name wolfram in English; they mention wolfram only to explain the symbol W.

There seemed to be a distinct lack of publicity about the book, which will be discussed at the CPEP meeting next week. CPEP has an Open Meeting on Monday, August 6, 2007. Publicity of IUPAC books seems to be between Dr Jost and the publisher. It was suggested that the whole Red Book be put on the IUPAC website.

13. Publicity

13.1 Translations

13.1.1 German translations of IUPAC documents. Since 2002 the journal *Angew. Chem.* has been publishing translations of IUPAC Recommendations of IUPAC Recommendations and technical Reports into German (see Appendix VII to the minutes of the Division Committee Meeting in Beijing for an extended list of published translations). Four translations were published in 2005 and four more in 2006. In 2007 two more translations have been published dealing with polymer terminology. The 2005-2007 translations are listed in Appendix VI.

13.1.2 A Spanish translation of the *Nomenclature of Inorganic Chemistry, IUPAC Recommendations 2005*, is available: *Nomenclatura de Quimica Inorganica. Recommendaciones de la IUPAC de 2005*.

13.2 IUPAC and IUBMB Website at Queen Mary College. Dr Moss distributed the statistics reflecting the usage of this website as of April 27, 2007. They are attached as Appendix VII.

13.3 IUPAC Website.

13.3.1. An article "IUPAC Web Developments" by Dr. David StC. Black, the IUPAC Secretary General appears in *Chem. Int.* **29**(4), 2–3 (2007).

13.3.2 The IUPAC Website is up and running in Berlin. All software development is being done in Prague. The back issues of *Pure Appl. Chem.* are being added to the Website. PAC is being digitalized in Prague and the entire PAC should be on the IUPAC Website by the end of 2007.

13.3.3 CPEP plans to contract out the work to take all the chemical structures from Volume 1 of PAC and add the IUPAC InChI/InChIkey to all articles.

13.4 Division VIII Webboard.

13.4.1 The current Division VIII Webboard is located on the RSC Website and is only one of many Webboards operated by RSC. The Division VIII Webboard will close at the end of the year. At least its equivalent is needed on the IUPAC Website. The type of interactive site used by the project group on graphic structure representation is good for individual projects, but is not set up for interactive participation. A Webboard on the IUPAC Website should operate across Divisions. Division VIII should have at least one person responsible for a Webboard that would serve Division VIII. A request should be made to CPEP to establish a project that will provide for setting up and operating a Webboard for Division VIII on the IUPAC website. Mr Brecher was asked and he agreed to take charge of our Webboard.

13.4.2 FIZ-Chemie, Berlin will provide Division VIII with the needed software for the Division VIII Webboard.

14. Reports from Other Committees

14.1 Committee on Chemistry Education (CCE).

14.1.1 Prof Hartshorn, our liaison with CCE, noted that there was nothing to report from the last meeting of this Committee. CCE will meet here in Turin Monday, August 6.

14.1.2 Prof Peter Mahaffy, Chairman, and Prof Eva Åkesson (Secretary) from CCE visited the Division VIII Committee meeting to talk about their projects and to ask for ideas from Division VIII.

14.1.3 Prof Leigh requested input from CCE with regard to the new edition of *Principles of Chemical Nomenclature, A Guide to IUPAC Recommendations*

14.1.4 Dr McNaught asked advice on how to get the recommendations on graphical representation of structures out to the public.

14.2 Committee on Printed and Electronic Publications (CPEP). This Committee will hold an Open Meeting on Monday, August 6, 2007

14.3 Committee on Chemistry and Industry (COCI). Within IUPAC COCI is the focus for issues of importance to the global chemical industry. More than 100 companies have joined with IUPAC as Company Associates. Dr Moss will replace Dr McNaught Division VIII's liaison on this Committee.

14.3.1 Dr Mark Cesa. Chairman of COCI visited with the Division Committee at 11:00 on August 4, to talk about how COCI and Division VIII can benefit each other.

14.3.2 Dr Moss noted the need for the Division Committee to have representation from industry. Over the years there have not been many members from an industrial setting on IUPAC Nomenclature Commissions (now Division VIII) but the chemical industry represents an important group of users.

14.3.3 Industrial chemists need to be included on the Advisory Subcommittee.

14.3.4 On the basis of a survey of Company Associates, it seems that industrial chemists acknowledge what we do in nomenclature matters and about InChI, but they do not want to read.

14.3.5 In order to get more companies involved it is necessary to have a wide influence, perhaps through the National Adhering Organizations, which are accessible through the Secretariat.

14.4 PAC Editorial Board. Dr Moss will replace Dr McNaught as Division VIII's liaison on this board.

14.5 Interdivisional Committee on Terminology, Nomenclature, and Symbols (ICTNS) Prof Nyitrai is a member of this Committee and can look after Division VIII interests.

15.0 Other Business

15.1 Dr Powell noted that a request had been received to provide an adequate definition of the term ‘polyamines’.

16.0 Next meeting. Dr Hellwich invited the Division Committee to meet in the vicinity of Frankfurt, probably in Büdingen, during the period July 28 – August 2. Details will be provided as soon as possible.

Submitted by: Warren H. Powell, Secretary, December 1, 2007.

Approved at the Division VIII Committee meeting in Büdingen, Germany, on July 31, 2008.

Appendix I

Correspondence with Dr G. A. Eller

Date: Wed, 26 Jul 2006 13:29:38 -0500
From: "John W. Jost" <secretariat@iupac.org>
Subject: Fwd: manuscript submission to PAC
To: "Jack W. Lorimer" <lorimer@uwo.ca>, Bernardo Herold <herold@ist.utl.pt>

Dear Jack & Bernardo,

How would you like to handle this. If you think the ms. has value it could be reviewed by Division VIII as a Technical Report, as was done with the Oman ms. Please let me know your decision

Regards,

John

> From: "Gernot A. Eller" <gernot.eller@univie.ac.at>
> To: <secretariat@iupac.org>
> Subject: manuscript submission to PAC
> Date: Wed, 26 Jul 2006 17:48:04 +0200
>
> To whom of the PAC editorial office this may concern,
>
> attached to this e-mail you find a manuscript on systematic nomenclature.
> Although I read that 'Unsolicited manuscripts are not normally considered
> for publication' I send this paper for publication in PAC as it seems to
> be well-suited to this journal, e.g. as a special topic paper.
>
> Initially, a previous version of this scholarly manuscript was submitted
> to the Journal of Chemical Information and Modelling (JCIM; assigned
> editor Dr. Wendy Warr, wendy@warr.com, who may be contacted for further
> information or for the referees' reports of manuscript ci-2006-00199m) and
> unfortunately found to be inappropriate for JCIM—although accepted (twice
> with minor corrections) and rated high from three of four referees. The
> fourth, rejecting referee suggested that the IUPAC journal would be a
> better home for this topic and the same advice was sent to me by e-mail
> from one of the accepting referees as he was informed by the editor of the
> manuscript's rejection. So, I came up with this journal.
>
> Due to (IU)PAC's traditionally strong connection and association to
> systematic nomenclature, which is outlined by the great number of
> published papers and reports with impact on this topic in PAC, this
> manuscript seems to be well-fitting to PAC, too. On the one hand, in this

> paper the nomenclature knowledge of the average chemists is analyzed, and
> on the other, methods for better and more correct application of the IUPAC
> nomenclature rules are given and discussed.

>
> Thus, the major outcome is, that chemical software can help very much both
> nomenclature experts and 'normal' scientists in the generation of a
> correct systematic name. Moreover, these software tools seem to be
> suitable for educational purposes as they greatly assist the learning and
> understanding of systematic nomenclature. Indirectly, these results
> advertise the importance of the union on systematic nomenclature.
> Hence, I am convinced that this paper should be regarded for publication
> in PAC.
> I am looking forward to hearing from you.
> Yours faithfully,

> Gernot Eller

> University of Vienna
> Department of Drug Synthesis
> Althanstraße 14
> A-1090 Vienna
> Austria
> e-mail: gernot.eller@univie.ac.at
> tel: ++43-1-4277-55634
> fax: ++43-1-4277-9556

International Union of Pure and Applied Chemistry

Division VIII

Chemical Nomenclature and Structure Representation

Please reply to:

Department of Chemistry
Queen Mary
University of London
Mile End Road
London E1 4NS

g.p.moss@qmul.ac.uk

Dr G.A. Eller
Department of Drug Synthesis
Faculty of Life Sciences
University of Vienna
Althanstrasse 14
1090 Vienna
Austria

13 October 2006

Dear Dr Eller

Improving the quality of published chemical names with nomenclature software

The above paper, which you sent to *Pure and Applied Chemistry*, has been sent to me as President of the Division concerned with chemical nomenclature. The Division has considered it and think that it has much merit and should be published somewhere. Unfortunately *Pure and Applied Chemistry* only publishes plenary lectures from IUPAC Symposia, recommendations and technical reports. Your paper does not come into any of these categories. To become a technical report it would need to have an international project to prepare the report. After wide-ranging discussions the best we can suggest is that you prepare a brief summary to be published in *Chemistry International* with a link to a full version on your website. Alternatively you might prefer to approach another journal.

Before publication we would require a number of changes. The first, and most important, would be to provide an IUPAC name for each compound discussed. There were suggestions that CAS names could be omitted.

It was felt that AutoNom should be mentioned as the first public program but it should be noted that it is no longer being developed and that it had a major error in that the priority of indicated hydrogen versus principle functional group is wrong.

The emphasis should be on software versus manual name generation, rather than between software companies. It was also felt that it should be emphasised that, after computer name generation, the output should be checked manually as programs are not infallible.

In the introduction other name-generating programs should be mentioned. Openeye software Lixichem and Bio-Rad NameItAll were sugested.

There were a number of trivial errors but if the manuscript is to be modified for publication the revised version should be reviewed by the Division again and these errors can be dealt with then. The review by the Division is important to ensure that the names comply with the IUPAC rules.

Yours sincerely,

G P Moss

President Division VIII

Appendix II

Nomenclature Committee of IUBMB (NC-IUBMB) and IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN)

Minutes of the Annual NC-IUBMB and JCBN Nomenclature Meeting

Chevy Chase, MD, May 5-6, 2007

Attendees:

NC-IUBMB and JCBN

Richard Cammack (London, UK)
Keith Tipton (Dublin, Ireland)
Hans Vliegenthart (Utrecht, The Netherlands)

NC-IUBMB

Dietmar Schomburg, Chairman (Braunschweig, Germany)
Helen Berman (Piscataway, NJ, USA)
Minoru Kanehisa (Kyoto, Japan)

JCBN

Sinéad Boyce, Secretary (Dublin, Ireland)
Gerard Moss (London, UK)

Others

Derek Horton (Washington, DC, USA)	Associate Member of NC-IUBMB
Alan McNaught (Cambridge, UK)	Associate Member of JCBN
Kristian Axelsen (Copenhagen, Denmark)	Observer
Sabine Kuhn (Columbus, OH, USA)	Observer

1. Welcome and Apologies

Cammack thanked Horton on behalf of the committees for making such excellent arrangements for the meeting. Apologies were received from Apweiler, Cantor, Chester, Cornish-Bowden, Degtyarenko, Dixon, Hellwich, Kazic and Nicholson

2. Approval of Agenda

It was agreed that the Chairman's report would be followed by Item 11 (a discussion of future projects) and that the presentations (Item 8) would be moved to the end of the meeting. With these modifications, the agenda was approved.

3. Minutes of the Bonn Meeting, May 2006

The minutes of the Bonn meeting were approved.

4. Matters Arising

None

5. Reports

5.1 Chairman's Report (Schomburg)

Schomburg reported that he had attended the IUBMB General Assembly, which was held in Kyoto in July 2006. As Kanehisa had kindly invited him, he did not have to use IUBMB funds for the trip. He said that there had been some discussions on our activities. In general, the comments were not very critical but a couple of points were raised. One was that there are a number of characterized enzymes that are not in the Enzyme List. He informed those who raised this issue of the methods for submitting details of unclassified enzymes so that they could be included in the Enzyme List. Another point raised was that we are a biochemical-nomenclature committee and not just an enzyme-nomenclature committee and therefore we should be working on other projects, with protein families being the most strongly felt need. This was discussed further under Item 11.

Schomburg said that a number of decisions were taken last year that concerned the database version of the Enzyme List (enzyme-database.org). He said that he was happy with the speed with which these decisions had been implemented in the database after the meeting. After discussions last year, Tipton, Boyce, Apweiler and Schomburg had agreed to a new arrangement to ensure that the IntEnz database contained an accurate copy of the Enzyme List from the Dublin database. Schomburg's group has started to write software to determine the differences between the two datasets and these will be sent on a regular basis to Axelsen, who can either accept the Dublin version or query its correctness. The software is almost completed but it has not yet been implemented. Schomburg reported that the Dublin database, from which he automatically downloads material for Brenda, is very straightforward, easy to understand and non-redundant. In contrast, IntEnz has a more complex structure and includes tags, which complicates the comparison process. For this reason, it is necessary to remove the tags (but retain the information) before comparing the two datasets. Once this has been done, the tags have to be re-entered. This imposes the restriction that each tagged item remains unchanged.

Schomburg has had discussions with Matthew Toussant, of CAS, who visited him in March 2007. They put together a number of points that they would like to proceed with in the form of a letter of agreement. This letter was distributed with the agenda and it was agreed to be a welcome development (**Action:** Schomburg to sign a letter of agreement with CAS).

Schomburg reported that an enzyme sub-committee meeting had taken place on May 4 and reported the major decisions that had been taken that need approval from the main meeting. These were as follows:

1. It was agreed that the use of more than one reaction equation in the Enzyme List will be restricted to cases where (1) the overall process involves sequential reactions or (2) a spontaneous reaction is involved in forming the reaction product(s). In cases where reactions are given that include alternative substrates, only the general reaction or one example will be used in the reaction field and the other reactions will be placed in a separate field that the user will have an option to view (**Action:** Boyce to modify those entries that contain multiple reactions where alternative substrates are given and Andrew McDonald to include a new field in the database to accommodate the specific examples).

2. It was decided that reactions should be mass-balanced but not necessarily charge-balanced.

3. Schomburg will approach the curators of databases that make extended use of EC numbers, reaction data etc. and ask them to include an acknowledgement that indicates that these data are from the IUBMB Nomenclature Committee. The wording of this acknowledgement is to be decided by Schomburg and Boyce (**Action:** Schomburg to draft acknowledgement and to consult database curators having finalized wording with Boyce; Boyce to send Schomburg a list of databases that use the JCBN data extensively).

The committees gave their approval for each of these.

3.2 Treasurer's Report (Cammack)

Cammack reported that we have funding from IUBMB and IUPAC. IUPAC funds JCBN titutlar members and IUBMB funds all other titular members. Whereas IUPAC funds travel costs plus a per diem, IUBMB currently reimburses for expenses based on receipts. IUBMB plans to use a similar formula to IUPAC but, for now, titular members should submit their expenses to Prof. Jan Joep H. H. M. de Pont (J.dePont@ncmls.ru.nl). They should also let Cammack know the amount claimed. Schomburg asked how quickly Cammack is informed about the amount of money claimed and he said that it was usually within a few days.

6 Enzyme Nomenclature and Classification

6.1 Progress report on the classification of enzymes and dissemination of enzyme data (Boyce, Tipton)

Tipton reported that the Newsletter was discussed at the enzyme sub-committee meeting, which was attended by Cammack. It was suggested, and agreed, that the newsletter, which Cammack is currently compiling, will be the final newsletter and that each item will be attributed to the person who suggested it. Thereafter, items will be published on an individual basis.

It was agreed at the last meeting to consider reclassification of EC 3.1.27.5 (pancreatic ribonuclease) as a lyase rather than remain as a hydrolase. The problem is that pancreatic ribonuclease catalyses a reaction in which a bond is not broken but is transferred to a different position to form a cyclic derivative (2,3-cyclic), which is hydrolysed to produce the product. The enzyme is responsible for the

internal transfer, i.e., it results in the formation of the cyclic derivative and then releases it. It is only when the enzyme has run out of all other substrate that it uses H_2O so it is essentially a lyase that acts as a hydrolase to produce its final product. Usage of the EC number 3.1.27.5 is widespread so changing it would cause problems. Tipton suggested that the enzyme should remain where it is but that the comments should be amended to indicate the enzyme's mechanism of action. The modified comments and a draft diagram of the mechanism for inclusion were presented. The entries for EC 3.1.27.1–4, EC 3.1.27.9 and EC 3.1.27.10, which appear to behave similarly, would also be amended. Berman said that she would strongly support Tipton's proposal and the meeting agreed.

Regarding the energases, Tipton requested approval for the version of the document that he presented last year in which the enzymes changing macromolecular conformation would be put in class 5.6, with, at present, two subclasses for (1) those acting on polypeptides (5.6.1) and (2) those acting on polynucleotides (5.6.2), regardless of whether or not the reaction involved NTP hydrolysis. This would entail the transfer of a number of the ATPases from subclass EC 3.6 to a new subclass 5.6. He has also prepared entries for a number of helicases and is to have a meeting in St. Andrews with John Somerville, who is an expert on dead-box helicases. The new material is ready to undergo internal review and could be distributed if members of the Committees wanted to see them. Otherwise they can be seen during public review.

Tipton reported that we have received a number of queries of the kind 'are these two enzymes the same?' or is 'enzyme x different from enzyme y?'. He said that to answer such questions required a good deal of literature review and it was often impossible to say. McNaught suggested that we have a standard reply to encourage the submitter of such questions to investigate the issue themselves.

Boyce reported that they had continued to amend the Enzyme List and had made a number of improvements to the database, as suggested by Schomburg at the 2006 meeting. These included making a public version of the log file and the inclusion of private notes indicating the changes made to each enzyme entry, along with the date and reason for the change. In addition, a frequently asked questions (FAQ) document was produced and is available at http://www.enzyme-database.org/faq.php.

6.2 Update on amine oxidases (Tipton)

The names that are ascribed to the two enzymes EC 1.4.3.4 and EC 1.4.3.6 do not follow our usual rules, which are to name enzymes according to the reaction(s) that they catalyse and not by their cofactor requirements. The reason for departure from the rules was that EC 1.4.3.4 and EC 1.4.3.6 were originally distinguished as monoamine oxidase (MAO) and diamine oxidase (DAO, also known as histaminase). Those names were changed when it was found that MAO could catalyse the deamination of some diamines, and that DAO from some sources was active towards monoamines but had little activity towards histamine. In fact, EC

1.4.3.6 contains a group of quite different enzymes, which have little in common except their sensitivity to inhibition by carbonyl-group reagents, such as semicarbazide, which does not inhibit EC 1.4.3.4. The correct course of action would be to delete EC 1.4.3.6 and create three new entries, although this would be very unpopular with those working in the amine-oxidase field. Tipton proposed that EC 1.4.3.4, amine oxidase (flavin-containing) be renamed as monoamine oxidase and that EC 1.4.3.6 amine oxidase (copper-containing) be deleted and replaced by two entries: one for primary-amine oxidase and the other for diamine oxidase. He has passed his proposals to Boyce for inclusion in the Enzyme List.

6.3 Publicity and information.

Not discussed

7. Items for Discussion

7.1 Standardization of the way that locants are indicated in chemical names – one year on. (Dixon, Moss and McNaught)

Last year we agreed to use a single system to indicate locants. This meant changing the way that locants were written for amino acids so that they matched that used for carbohydrates, e.g. N^6- became 6-*N*-. This change was implemented in the enzyme database, since it was understood that such a system would have the support of IUPAC. However, that turned out not to be the case. Boyce and Schomburg recommended that we revert to the old system and this was agreed. (**Action:** Boyce to undo all changes made to locants for amino acids in the Enzyme List)

7.2 Contributions for the forthcoming new edition of Jeff Leigh's "Principles of Chemical Nomenclature" (Cammack)

Cammack raised the subject of a request by Jeff Leigh for suggestions for items to be included in the second edition of “Principles of Chemical Nomenclature”. This book, published by IUPAC, offers an accessible introduction to nomenclature for students. It includes an explanation of how a range of common types of compound are named, and why. The book can be downloaded as a PDF file from http://www.iupac.org/publications/books/principles/principles_of_nomenclature.pdf. Moss and Dixon are responsible for revising the biochemical section for the new edition of the book. Moss would like suggestions about what should be included that is not present in the current version (**Action:** those with suggestions to pass them on to Moss).

7.3 Discussion of papers by Sobkowski *et al.* on proposals for denoting stereochemistry for P-chiral nucleotide analogues. (Moss, Dixon)

Moss said that he could see why the authors Sobkowski *et al.* wanted more specific stereochemical descriptors but said that he was not convinced of the value of their proposed system of using *D* and *L*. Vliegenthart said that the proposals of Sobkowski *et al.* would not be accepted in the chemical community. Moss said that he would prefer to stick to the *R/S* system, but noted that it was not easy to define how to apply *R* and *S* to a phosphorus atom. Some phosphorus atoms have random

configuration whereas others are controlled, e.g. *all-R* or *all-S*. For the case with random configuration, Dixon had suggested that the term '*all-ambo*' could be used and Vliegenthart said that he would have no objection to this. Vliegenthart asked if a decision should be made at the meeting and suggested that this issue could be covered by a newsletter item.

7.4 Need for a term to describe the relationship of the various ionic and neutral forms of a multifunctional compound with each other. (McNaught)

ChEBI incorporates a classification system for small molecules that describes the relationship between the constituents in the database. There is no term to encompass all the forms of a multifunctional compound that can exist in a number of protonation states. 'Conjugate acid' and 'conjugate base' can be used for a matched pair where one proton is involved but cannot be used to describe a group of compounds such as phosphate in its various protonation states. McNaught suggested that the word 'alloprote' be used to describe such a situation but Tipton disliked the term saying that it might be confused with the term 'allotrope'. If anyone has an alternative to alloprote, they are to inform McNaught. To bring the issue to the wider community Moss suggested raising it in a Chemical Information Sources Discussion List (CHMINF-L) e-mail (**Action:** anyone with a suggested alternative to alloprote to contact McNaught; Moss or McNaught to send a CHMINF-L e-mail on the subject).

7.5 Approval of the phosphorus document so that it can be submitted to IUPAC (Dixon, McNaught)

Vliegenthart commented that the phosphorus document was a very impressive and well-written document. Moss had one comment to make, which related to the naming of antisense oligonucleotides (Item 9.21 of the agenda). Sabine Kuhn had brought along examples of how CAS handles the problem of naming antisense oligonucleotides and Moss wondered if this should be included in the phosphorus document even at this late stage. As Moss only received the information at the meeting he said that he will circulate recommendations within the next month or two. McNaught suggested that it be added to the IUPAC web discussion board, which would be part of the review process anyway. The phosphorus document was accepted as it now stands and the committees will comment on other changes by e-mail (i.e. will not wait until the next meeting to give final approval). (**Action:** Moss to circulate recommendations for naming antisense oligonucleotides to be included in the phosphorus document and the committees to send him comments on his recommendations by e-mail).

7.6 Inconsistencies in enzyme data between the data on the qmul website and at enzyme-database.org (Axelsen)

Axelsen provided a document containing some discrepancies between the enzyme data on the qmul website and at enzyme-database.org. Among these were differences in formatting of subscripts, missing CAS numbers from the database version and implementation of the change to locants in the database but not in the qmul files. Tipton said that it would have been helpful if Axelsen had sent this list

directly to Boyce so that the discrepancies could have been rectified, but Axelsen said that it was not his job to find discrepancies between the IUBMB pages and ExplorEnz. Boyce said that there were various reasons for these discrepancies and Schomburg pointed out that the new systems now in operation should minimize any discrepancies but Axelsen said it was unacceptable for there to be any at all. Schomburg suggested that there should be software to compare the two datasets and indicate differences and this was agreed. (**Action:** Schomburg's programmer/students and Andrew McDonald to work on the production of software to compare the datasets).

7.7 Membership of Committees

Schomburg said that this item has two parts: (1) the large number of titular and associate members but the limited scope of projects and (2) a proposal he received from Berman concerning the membership of database representatives. Schomburg suggested that we make sure that all members of the groups (both titular and associate members) are involved in a nomenclature project. He asked if anyone was opposed to this and there were no objections. Tipton said that it was essential that we address this issue as the IUBMB had raised it as a matter of concern. (**Action:** Schomburg to compile a list of projects that will be published on the website along with the members involved in each project).

Schomburg said that the databases made a valuable contribution to the Enzyme List. He reported that, since May 2006, 1087 out of the current 4015 enzyme entries have had minor changes made to them. He said that BRENDA had provided proposals for 107 new EC numbers, 30 modifications to existing entries, 44 corrections and 11 minor corrections. SIB had provided proposals for approximately 30 new enzyme entries and numerous minor corrections. Tipton said that MetaCyc had also been most helpful in this respect. Schomburg asked Kanehisa and Berman to send details of new enzymes that they find with their databases (along with associated references) to Boyce for inclusion in the Enzyme List. Kanehisa said that he would try to do this. When asked, Berman said that she was not sure if they came across unclassified reactions in PDB but she expected that they would in the near future. She said that they would need to have a formalized procedure for her annotation staff to incorporate into their work schedules. Schomburg suggested that they send a message every three months with lists of enzymes and associated references. Berman said that someone should send her a formal letter saying what is required that will be circulated worldwide. It was noted that all committee members should send data on unclassified enzymes to Boyce if they come across them. Moss referred to Janet Thornton's database EC -> PDB (http://www.ebi.ac.uk/thornton-srv/databases/enzymes/) , which is used to link enzyme entries to the relevant PDB entries. Berman agreed that it would be helpful to provide links to that. (**Action:** Boyce to draft letter; Axelsen and Berman are to coordinate the data that they will send to Boyce; Kanehisa to send new enzymes plus associated references to Boyce for inclusion in the Enzyme List).

Berman suggested that instead of having titular or associate membership for team leaders of major databases, it would be better to assign a kind of associate membership to the database itself so that nomenclature meetings could, if appropriate, be attended by someone other than the team leader. This proposal did not exclude the possibility of titular membership remaining for those who would prefer it. This would represent a change to our standard procedure so that the wording on the membership page of our website could be changed to something such as 'representative of PDB' rather than naming Berman personally. McNaught suggested that such memberships should be reviewed regularly to ensure that they remain appropriate. This was agreed, and Schomburg suggested revision every three years. The databases presently concerned are PDB, KEGG, BRENDA, UniProt and CAS . Horton suggested that Oxford Glycoscience be included. Axelsen reported that GlycoSuiteDB was no longer in operation. EuroCarb might also need to be included (http://www.eurocarbdb.org/; James Paulson is lead on this NIH-funded project). He may be invited as an observer to the meeting next year. It was also suggested by Horton that Bernard Henrissat from CAZy (http://www.cazy.org/; Carbohydrate-Active Enzymes) be invited to the next meeting as he has been critical of the Committees' work. Moss suggested three membership categories: Titular, Associate and Database Representative and this was agreed. Tipton suggested that Ron Caspi be invited as a representative of MetaCyc (http://metacyc.org/) as he provides valuable enzyme data on an ongoing basis.

7.8 Proposed cooperative effort between CAS and NC-IUBMB (Schomburg, Kuhn)

The proposed letter of agreement was sent with the Agenda. Schomburg proposed that we accept the terms of the agreement and this was agreed. He will write a letter to Matthew Toussant to this effect. Sabine Kuhn said that they have downloaded the xml version of the enzyme database from Dublin and are looking through the data. They are checking the CAS registry numbers and have found some instances where we do not have the correct registry number or are missing it completely. They plan to complete the checking of data within the next few months and will sort out a method of collaboration (**Action:** Schomburg to write letter of agreement; Sabine Kuhn and Boyce to discuss details offline).

7.9 Possibilities for cooperation with the EPA (Cammack)

Cammack reported he had written to the EPA saying that we would be willing to assign EC numbers for new enzymes and that we could do this within their timeframe. They had intended to send an observer to our meeting but were unable to do so as it overlapped with another meeting. They said that they would like to see the minutes, in particular, the item on CAS. Moss said that the same criteria would have to apply to EPA enzymes as for other new enzymes. Sabine Kuhn reported that, from what she has seen, the EPA request a lot of data so it should be conducive to drafting entries.

7.10 Progress report on the work of the thermodynamic panel chaired by Bob Alberty (membership: Athel Cornish-Bowden, Hal Dixon, Robert Goldberg, Gordon Hammes, Keith Tipton and Hans Westerhoff)

Tipton reported that Bob Alberty disagrees with the practice of including any charges in biochemical reactions as we do not include all charges and we use them inconsistently. Having a chargeless equation would be useful for thermodynamics but would not allow us to mass-balance reaction equations. Tipton said that Alberty has produced a preliminary document. Some others on Alberty's committee have indicated that a majority of biochemists are less concerned about the strict requirements of thermodynamics and would not be happy to have all charges removed. They are hoping to get an IUPAC document finalized. Alberty would prefer the term 'reduced NAD' or '$NADH_2$' to be used rather than 'NADH'. The group is to meet later this year.

7.11 Publication of a newsletter

Cammack reported that he has been assembling items from past Minutes to include in the next newsletter. He said that he was not sure of the style of the newsletter as most items will not be in the form of rules, but will be more a list of things that we have done. Some of the topics he has collated include: bioinformatics, energases, recommended name, carbohydrate symbols, lipid classification, the phosphorus document, small molecules such as pyrrolysine, the use of gene symbols and the Blue and Red Books. He said that he will consolidate the list and then consult with committee members asking for input/feedback. Cammack said that he would do this on his return from the meeting. He said that he would like it to be published in IUBMB Life but will make it clear that it can also be published by other journals. Boyce said that this type of newsletter was a departure from our usual practice, which was to include only items that were recommendations on biochemical usage. It was agreed that the newsletter would be split into two documents: (1) recommendations and (2) a less formal part that provides details of our activities (**Action:** Cammack to compile list of topics to include in each of the newsletters and to consult with members of the committees about the content of these newsletter items).

8 Presentations

8.1 Progress report on cleaning reaction data and adding organism information in KEGG (Kanehisa)

Kanehisa reported that there was a distinction between IUBMB reactions and KEGG reactions. For each KEGG reaction, other reactions are given and he used EC 1.1.1.21 for demonstration purposes. There are 6807 reactions in KEGG's reaction database compared with 3222 in IUBMB data. They are using their RPAIR database to predict xenobiotic degradation pathways (paper in press in *J. Chem. Inf. Model* by Oh *et al.*, 2007). RPAIR is an integrated version of pathcomp and e-zyme and it may be used for automatic EC number assignment (first three numbers). Kanehisa said that organism information is required for gene annotation. He also said that it is difficult to assign genes to EC numbers as there could well be species differences etc. Kanehisa reported that some of the references cited in the Enzyme List are missing their PMID numbers and he will send Boyce a list of these missing PMIDs (**Action:** Kanehisa to send Boyce his list of PMID numbers to include in the Enzyme List).

8.2 New developments made within the IntEnz project: a reaction database called RhEA (Axelsen)

Axelsen reported on a new project in which they are trying to make a reaction database. He said that some of the reactions might seem redundant but that they will also provide crosslinking when there are parallel reactions. They intend to have reactions described by their compounds and are also trying to ensure that all compound names used in the IUBMB Enzyme List are consistent. They will also introduce additional reactions into the database and will link to a pathway description initiative in UniProt. Reactions are stored as plain text. Problems encountered include redundancy, ambiguity, isolation and instability. He said that 'people' do not like the EC number being used as a primary identifier as it can be changed. An example of inconsistent terms for the same compound is CoASH, CoA-SH, CoA, which are all used for coenzyme A. All compounds in the database will be linked to ChEBI. There is no interface to the database as yet. He also said that the UniProt protein-naming guidelines could be found at http://www.expasy.org/cgi-bin/lists?nameprot.txt.

8.3 Progress report on Don Nicholson's metabolic-pathway charts, minimaps and animaps (Tipton)

Tipton updated the committees on Nicholson's activities and showed Nicholson's recent animap of the mitochondrial respiratory chain.

8.4 Update on usage of Moss' IUBMB and IUPAC websites (Moss)

Moss provided the usage statistics for his website and said that they were much the same as for last year.

9 Update on Action Items from the Minutes of the 2006 Meeting

9.1 Dublin to include timestamps for all fields in which data have been modified (Minute 5.1: Action by Boyce, McDonald)

Done

9.2 Boyce to replace 'Common name', and 'Recommended name' for enzymes in EC 3.4, with 'Accepted name' (Minute 5.1: Action by Boyce)

Done

9.3 Boyce to distribute UniProt document with the Minutes (Minute 5.1: Action by Boyce)

Done

9.4 Moss to approach Chemical Abstracts regarding nomination of a representative to the Committees as an Associate Member (Minute 6.5: Action by Moss)

Done

9.5 Inclusion of acknowledgement on enzyme website of those offering significant advice on specific enzymes (Minute 5.1: Action by Schomburg and Moss)

We still need to come up with a list of people to include

9.6 Cammack to coordinate application for IUPAC funding of a project on small-molecule nomenclature (Minute 5.1: Action by Cammack)

This was discussed under Item 11.1

9.7 Schomburg to draft contract indicating that the database archive will be stored at the EBI but that the EBI cannot make any changes to the data in the database. However, they would be responsible for guaranteeing its long-term availability. (Minute 5.1: Action by Schomburg)

This has been deferred

9.8 Schomburg to inform IUBMB and IUPAC of decision to use the name 'Joint Committees on Biochemical Nomenclature' as an umbrella term for the JCBN and NC-IUBMB committees (Minute 6: Action by Schomburg) (**Action:** Schomburg will send the relevant information to Moss to pass on)

9.9 Ida Schomburg to revise data on new peptidase enzymes and Boyce to draft entries (Minute 7.3: Action by Ida Schomburg and Boyce).

This is in progress with many of the entries having been made official

9.10 Tipton to contact David Lilly to ask him if he would act as an expert on nucleic-acid-related enzymes and Kazic to contact other possible experts (Minute 7.3: Action by Tipton and Kazic)

Tipton has now consulted with Lilly and others who said that there were various subfields within the general term 'nucleic-acid-related enzymes' so that we would need different people to advise on each of them. Lilly did not want to participate personally.

9.11 Boyce to include an explanation of why accepted names are sometimes changed in the FAQ document and Tipton to inform Prof. Kyte of the decision reached (Minute 7.4: Action by Boyce and Tipton)

Done (available at http://www.enzyme-database.org/faq.php)

9.12 Schomburg, Axelsen, Apweiler and Kazic to determine if there are any reasons not to implement Karp's recommendations for distinguishing between partial EC numbers; Schomburg to discuss the proposal with people from The EMBL Nucleotide Sequence Database, KEGG and UniProt, and Moss to include a note on the proposal on his website along with a request for feedback (Minute 7.6: Action by Schomburg, Axelsen, Apweiler, Kazic and Moss)

Apweiler had reported that UniProt was happy with Karp's recommendations although they have decided not to use the '?' symbol but to continue to use the hyphen for cases where an enzyme most probably exists but has not been characterized sufficiently to warrant an EC number ('n' will be used when the enzyme has been characterized, as recommended by Karp). (**Action:** Schomburg will report on this to Peter Karp).

9.13 Tipton to send Boyce his revised list of isomerases that are energases for inclusion in the Enzyme List (Minute 7.7: Action by Tipton)

Done

9.14 Boyce to reclassify EC 3.1.27.5, pancreatic ribonuclease as a lyase (Minute 7.9: Action by Boyce)

See item 6.1

9.15 Cammack to continue discussions with the EPA regarding the provision of EC numbers for enzymes and remuneration for this activity. (Minute 8.2: Action by Cammack)

This was discussed under Item 7.9

9.16 Schomburg to notify IUPAC and IUBMB of the change to the way that locants are written for amino acids and Boyce to implement the associated changes in the Enzyme List; McNaught to draft a corrections notice on the subject of locants for publication in Pure and Applied Chemistry. Once approved by the Committees, this will need to go through the IUPAC review procedure before final approval (Minute 8.4: Action by Boyce, Moss, Schomburg and McNaught)

This change to the way locants are written for amino acids was implemented by Boyce but, following the decision taken under Item 7.1, is now obsolete so Boyce is to revert to the previous way of writing locants.

9.17 Moss, McNaught, Hellwich and Dixon to draft recommendations on how to indicate doubly substituted peptides (Minute 8.5: Action by Moss, McNaught, Hellwich and Dixon)

Hellwich sent his proposed recommendations to Boyce, McNaught and Moss in August 2006 and said that he hoped to discuss the matter with McNaught and Moss

9.18 Boyce to draft a Newsletter item on the use of the letter 'O' as the one-letter code and 'Pyl' as the three-letter code for pyrrolysine (Minute 8.6: Action by Boyce)

Done

9.19 Cammack to send further details of his talks with the IUBMB and Richard Roberts regarding possible new associate members to join the committees (Minute 9.3: Action by Cammack)

Membership of the committees was discussed under Item 7.7

9.20 Schomburg will contact von der Lieth (carbohydrate expert) and invite him to our next meeting (Minute 9.18: Action by Schomburg)

Schomburg said that he forgot about this but will approach Bernard Henrissat to see if he will come to the meeting next year (**Action:** Schomburg to invite Bernard Henrissat to the 2008 meeting as an observer)

9.21 Sabine Kuhn to contact Moss about procedure used at CAS and Moss to contact Berman's associate regarding how PDB handle the problem of naming antisense oligonucleotides (Minute 9.24; Action by Kuhn and Schomburg)

Done

9.22 Schomburg to consult with the IUBMB Executive to discuss the possibility/viability of producing a new edition of the Enzyme Nomenclature book (Minute 9.27: Action by Schomburg)

Angelo Azzi said that he would endorse the publication of a new edition of the book if we wanted to go ahead with this. He made three stipulations: (1) copyright would remain with the IUBMB (2) if there was a loss on the publication, the publisher would stand the cost and not the IUBMB and (3) the royalties would go to the IUBMB but the market value would be set by Elsevier.

This is still open

9.23 Interested parties to submit suggestions to Horton regarding sections of the carbohydrate document that should be revised (Minute 11.2; Action by all interested parties)

Ongoing

9.24 Boyce to collate items for a newsletter and Schomburg to consult with the Executive Committees about publishing a condensed version of the Minutes (Minute 12.1; Action by Boyce and Schomburg)

Cammack wished to coordinate the newsletter

9.25 Schomburg to make request to the IUBMB for online access to BAMBED (Minute 15.1; Action by Schomburg)

Schomburg did not get a response so will try again (**Action:** Schomburg to request online access to BAMBED again)

10 Funding Situation and Possibilities (Cammack, Moss)

Schomburg submitted an application to Beilstein in 2006 for funding for enzyme work and the application was looked upon favourably. A final decision should have been made last October but the Beilstein database is being bought by Elsevier so the situation is uncertain. Royalties from the Beilstein Institute used to be used, amongst other things, to fund database activities but they are unsure what is going to happen now. The situation should be clearer in October 2007. There is the possibility of getting funds from IUPAC via projects but no funding possibilities from IUBMB. ESFRI, The European Strategy for Research Infrastructure, was suggested as a possibility for funding. Janet Thornton has put in a major application for such funding. Research Infrastructure is to be funded on a long-term basis but the whole Framework process takes four years so there would no funds for at least four years If the application to Beilstein does not work out, we could try another private fund. National bodies do not appear to be interested in funding an international effort and the European Union generally only supports larger projects. The Wellcome Trust was suggested as a possibility.

11 Future Projects and Activities

11.1 Revision of carbohydrate nomenclature (Horton)

To address the criticism that we are concerned only with enzyme issues, Moss suggested that we assign projects to different members of the committees and make this information available on our website. Schomburg asked if there were any high-priority projects that we should start immediately. McNaught said that we do not address the issue of general biochemical terminology and Tipton said that this would be very useful.

Carbohydrate document: Schomburg asked for the status of the revision of the carbohydrate nomenclature. Horton said that the 1996 document is over ten years old, but has had small corrections incorporated in the web version. He said that there was no urgent reason to do a major revision as it covers all areas, including synthetic organic chemistry. Biochemists do not need such a detailed document. Instead, they require a more simplified document that addresses rapidly developing areas of biochemical interest, such as glycolipids, glycoproteins and glycosaminoglycans. Horton has started the process of producing a carbohydrate document for biochemists by removing all material that would be of interest primarily to organic chemists. He said that there may still be more information in the document than biochemists would need. He suggested that some permitted biochemical usages be included and that the area of polysaccharides and glycoproteins may need some amplification by adding examples. The document is still at a preliminary stage but he would appreciate comments and suggestions of areas where biochemists do need the information currently contained in the document (**Action:** Moss to distribute the document to members of the mailing list who are to make suggestions to Horton).

Moss asked if this work comprises two projects rather than one, with the first being a concise document for biochemists and the second an update of the carbohydrate document. He pointed out that corrections to the 1996 version had been made to the web version but that they need to be published. Moss said that he was most

concerned with polysaccharides, where the rules for naming them are not given and this makes it difficult to name all but the simplest polysaccharides. The document also lacks guidance on naming repeating monosaccharides. The second document should be covered by a supplement to the 1996 document rather than a complete rewrite (**Action:** Horton, Vliegenthart, McNaught, Dixon and Moss to work on the supplement to the 1996 carbohydrate document). The resulting supplement will need to be submitted as an IUPAC project proposal to have IUPAC approval. It was not decided who would make the application. The documents (supplement and biochemists' version) are to be distributed to the mailing list three months prior to the next meeting (**Action:** Horton to send the supplement to the 1996 Carbohydrate document and the biochemists' version of the document to the committees by 8 February 2008).

11.2 Small-molecules project:

Schomburg reminded the meeting that this had been on the books since approximately 1998. This will be important as an extension of the glossary to cover small molecules of biochemical interest and to indicate the recommended names for a number of small molecules. In 2006, Cammack agreed to submit an application to IUPAC to obtain project status. Cammack said that he had collated some data and consulted with the subgroup but he was unsure of how this project would differ from ChEBI and PubChem and of the project's objectives. Therefore, he had not made an application to IUPAC for project approval and no further work had been carried out.

Moss said that, since the project was to compile a list of molecules of importance to biochemistry that have not been covered by other nomenclature documents, it is completely different from ChEBI or PubChem. Its aim would be to provide structure and numbering information for molecules such as thiamine diphosphate, riboflavin and coenzyme A that are very common but for which it is difficult to find such information. In order to compile the list of useful biochemical compounds McNaught suggested that the working group could compile a list of the small molecules that occur most often in the Enzyme List and determine if the top 100 are already covered. This should provide a good starting point. Cammack said that he would like to remain as coordinator and it was agreed that McNaught and Schomburg be added to the list of working-group members. The application is not to be submitted to IUPAC until the working group have an idea of the molecules to be included and a more descriptive title than 'small molecules'. Moss suggested that definitions of nucleic acids, nucleosides and nucleotides be included as these are difficult to find in our current recommendations (e.g. define adenosine, thymidine, etc.). Preliminary results should be circulated to the JCBN no later than three months prior to the next meeting. Berman said that someone from her group should play a leading role in this project as they had compiled a dictionary of small molecules (available at http://remediation.wwpdb.org/downloads.html and maintained by John Westbrook). She said that this dictionary contains all of the nomenclature and chemical characteristics, SMILES, synonyms etc. of all small molecules and monomer units within PDB. Each component also has a three-letter code. Berman said that they would need input from JCBN to ensure that they are acting correctly.

They want to make sure that there are no contradictions between our document and their database. (**Action:** McNaught, Schomburg and someone from PDB to be included in the working group, whose membership may need revision. Cammack to submit an application to IUPAC for project approval when preliminary investigations have been completed and to distribute the output to the committees by 8 February 2008).

11.3 Other protein classes:

We could draft a document on general guidelines for naming proteins using the UniProt document that was distributed with the 2006 Minutes as a starting point. Axelsen said that this work should be coordinated with SIB as they are also working on a similar document. The SIB document will have a broader scope. He reported that Amos Bairoch has written the first draft but Axelsen did not know who would coordinate the effort at SIB. (**Action:** Axelsen, Berman and Kanehisa to give this further consideration).

11.4 Transcription factors (TFs):

Schomburg knows of a group that have a database on transcription factors (TRANSFAC; http://www.gene-regulation.com/pub/databases.html#transfac) and they were invited to the meeting but could not attend. They classify TFs based on the first DNA binding domain. The database is updated frequently. Schomburg said that he would like them to come up with a proposal (paper) that should be finished by the end of year and that could be discussed at the next meeting. Tipton said that it would be good if the committees could collaborate with them. Berman asked if these were the primary people involved in TFs and Axelsen and Kanehisa said that this group had no competitors in the field so would be appropriate. Berman said that she would be happy to be involved at the beginning of this project. The document should be given IUBMB status and, if they agree, we could include E. Wingender as an Associate Member of the group (**Action:** Schomburg to ask TRANSFAC group to draft a paper on transcription factors)

11.5 Peptide hormones:

We have a very old document (1974; http://www.chem.qmul.ac.uk/iubmb/misc/phorm.html) to cover what is a very active area. Schomburg said that we should try to find someone who works in this area who might be able to update the document. Berman said that a group at NRL have common names for peptide hormones and that these are the names that people use. Moss said that there are people who need the correct chemical name and Berman replied that there is a way to obtain such names that is relatively straightforward. Berman stated that there is a nomenclature for peptide hormones (L-Ala-D-Leu etc.) but that common names are used. Tipton reported that neuroscientists often devised different name for peptides they found and subsequently found out that what they were working on was a peptide hormone. He said that having a common name, synonyms and sequence may be useful. Sabine Kuhn said that, in CAS, they have approximately 100 basic peptide names based on trivial names and then have more systematic names. Schomburg asked for

participants for a working group on peptide hormones and it was agreed to try to formulate the membership of the working group by the next meeting. Tipton volunteered to be a member of the working group, but not the coordinator.

12 Any Other Business

The attention of the meeting was drawn to the Ligraph tool to convert a sugar graph to ASCII IUPAC sugar nomenclature. This is available from http://www.glycosciences.de/tools/LiGraph/.

13 Date and Place of Meeting in 2008

The next meeting will take place on 17-18 May, 2008. Axelsen is to determine if he can host the next meeting in Copenhagen and will let us know within one month. If it is not possible, the meeting will be hosted by Schomburg in Braunschweig.

14 Open Forum

McNaught reported that InChI is going to comprise a hash algorithm that will provide random 18-character codes and will be available in July. He said that this will be easier for searching but will not be reversible. He expects that users will make their own collections and there has been positive feedback on this. He also reported that there has been a new arrangement of RSC journals whereby text mining has been used to enable users to access definitions provided by IUPAC and others. RSC recently introduced “Project Prospect”, which puts all new journal papers through a text-mining program, resulting in all users being able to highlight terms that have been defined by IUPAC, in the gene ontology and chemical names. The chemical names link will take the user to a structure, an InChI and a CML file. All of this is automated and is available from the RSC website (see http://www.rsc.org/Publishing/Journals/ProjectProspect/ for more details).

Appendix III

IUPAC International Chemical Identifier

Report to IUPAC Division VIII, August 2007

The IUPAC International Chemical Identifier (InChI) is a character string unique to a specified chemical structure, generated algorithmically and reconvertible into the original structure. For full details see www.iupac.org/inchi. It is now being used by a wide range of software and internet databases and by several primary journals: details are appended to this report.

1.0 Funding of Guest Researcher at US National Institute of Standards and Technology (NIST)

IUPAC is now partially subsidising a new Guest Researcher at NIST, working full time on InChI development alongside Steve Stein and Dmitrii Tchekhovskoi. He is Dr Igor Pletnev from Moscow State University. He arrived in February of this year and is currently familiarising himself with the details of the InChI algorithm and associated software, and working on modularisation of the software and development of the InChI 'hash' (see below). Future work will be devoted to extending the InChI application to simple polymers, Markush structures and excited states and other areas as time and resources permit.

2.0 InChI 'Hash' Algorithm

In informatics, a 'hash' is a character string of specified (short) length generated algorithmically from a string of variable length to facilitate data handling. The recently launched InChI hash has been developed to facilitate use of the InChI by web search engines, which break a long InChI
string in unpredictable ways. It consists of 20 characters (including a check character) plus two delimiter "-" signs, and separately encodes molecular skeleton and stereo/isotopo/tautomers. Although close to unique (hash collisions would not be expected with a dataset of less than 250 million molecular skeletons) it cannot be converted back to the original structure.

3.0 Assignment of Uniform Resource Identifier (URI)

A Uniform Resource Identifier (URI) provides a simple and extensible means for identifying a resource within the World Wide Web global information architecture. Each URI begins with a scheme name that refers to a specification for assigning identifiers within that scheme. As such, the URI syntax is a federated and extensible naming system wherein each scheme's specification may further restrict the syntax

and semantics of identifiers using that scheme. InChI has now been assigned a URI namespace: see

http://info-uri.info/registry/OAIHandler?verb=GetRecord&metadataPrefix=reg&identifier=info:inchi/

This will assist development of InChI web applications

4.0 InChI Publicity

Steve Heller has developed a programme of presentations and meetings to publicise InChI. Details are attached. The resulting take-up by a wide range of organisations (see appended lists) is very encouraging. However the take up by primary journal publishers is not yet widespread, although the impressive implementation by the Royal Society of Chemistry, including links to definitions from the IUPAC Gold Book and other databases may stimulate activity from other organisations:

http://www.rsc.org/Publishing/Journals/ProjectProspect/

IUPAC funding has now been approved for a further plan of meetings to encourage take-up by journal publishers and to publicise the facilities offered by the InChI hash (for example a further lecture to Google developers).

Alan McNaught

July 2007

InChI takeup by software developers, database providers, and journal publishers, July 2007

Software:

1. Structure Drawing

a. ACD Labs: ChemSketch www.acdlabs.com
b. CambridgeSoft: ChemDraw www.cambridgesoft.com
c. ChemAxon: Marvin www.chemaxon.com
d. BK-Chem: http://bkchem.zirael.org/inchi_en.html
e. CACTVS structure editor csed: www.xemistry.com/academic
f. PubChem Online Sketcher (based on CACTVS): pubchem.ncbi.nlm.nih.gov/edit
g. MDL: MDL draw www.mdl.com

2. Structure Search

a. IBM (internal project)
b. CACTVS structure search system www.xemistry.com/academic
(the technology behind PubChem structure search:
pubchem.ncbi.nlm.nih.gov/search and NCI's Chemical Structure Lookup Service:
http://cactus.nci.nih.gov/cgi-bin/lookup/search)

3. Analysis software

a. SciTegic: http://www.scitegic.com

4. Structure file interconversion

a. OpenBabel: http://openbabel.sourceforge.net/RELEASE.shtml
b. CACTVS system universal file converter csib: www.xemistry.com
c. Molecular Networks convert: http://mol-net.de/software/category/converting.html

5. Other software

a. World Wide Molecular Matrix: http://wwmm.ch.cam.ac.uk/gridsphere/gridsphere
b. CACTVS chemical scripting toolkit: www.xemistry.com/academic
c. InChImatic: http://inchimatic.com
d. Java Native Interface InChI Wrapper:
http://jni-inchi.sourceforge.net/

Databases:

1. NIST WebBook http://webbook.nist.gov
2. NIH PubChem http://pubchem.ncbi.nlm.nih.gov
3. NCI DTP http://cactus.nci.nih.gov/ncidb2/
4. EPA - DSSTox www.epa.gov/nheerl/dsstox/
5. UC-SF ZINC project http://blaster.docking.org/zinc/
6. KEGG www.genome.ad.jp/kegg/
7. ISI Web of Science http://portal.isiknowledge.com/
8. Carcinogenic Potency http://potency.berkeley.edu/structure.html
9. ChEBI www.ebi.ac.uk/chebi
10. Wiley Mass Spectra www.wiley.com/WileyCDA/Section/id-131370.html
11. Prous Science Integrity http://integrity.prous.com/integrity/servlet/xmlxsl/
12. FDA GeneTox and Chronic/subchronic Databases
www.leadscope.com/fdadb_cat.php
13. Compendium of Pesticide Common Names
www.alanwood.net/pesticides
14. ChemBank http://chembank.broad.harvard.edu
15. SPRESI http://infochem.de/en/products/spresiweb.shtml
16. Specs.net: http://www.specs.net

Journal Publishers:

1. Royal Society of Chemistry www.rsc.org/Publishing/Journals/ProjectProspect/
2. Prous Science - *Drugs of the Future*
3. BioMed Central - Chemistry Central www.chemistrycentral.com

InChI meetings/presentations by Steve Heller since 2005 IUPAC meeting in Beijing

1. Beilstein Institute seminar - Frankfurt, Germany - 11/05
2. Goslar Chemical Information conference lecture - Goslar, Germany - 11/05
3. PacifiChem Poster - Honolulu - 12/05
4. Federal Drug Administration Science Forum invited lecture - Washington DC - 4/06
5. Prous User Meeting invited lecture - Barcelona - 9/06
6. Google lecture - Mountain View, CA - 11/06
7. Prous User Meeting invited lecture - Tokyo - 3/07
8. Prous User Meeting invited lecture - Osaka - 3/07
9. American Chemical Society meeting - Chicago invited lecture - 3/06
10. NIST Physical and Chemical Properties Division laboratory invited lecture - Boulder, CO - 4/06
11. Various meetings with Wiley, Elsevier, ISI, and Knovel staff in Germany and New York
12. Meetings with CambridgeSoft and MDL staff at American Chemical Society conferences
13. Numerous meetings with National Institutes of Health-National Cancer Institute and PubChem staff – Washington DC
14. Meeting with Royal Society of Chemistry staff - 3/07
15. Meetings with Dr Henry Rzepa, Imperial College, London 12/05 and 3/07

Appendix IV

Meeting of Task Group 2006-029-1-800, Lingotto, Turino, 3 August 2007

The purpose of this meeting was to finalise details of the procedures and timetable for preparing the first version of the new edition (Principles 2). This should be circulated to all members of the Task Group by early May, 2008, in preparation for the next Task Group meeting in August 2008.

Outline Plan of pattern of work tasks for Project 2006-029-1-800

(Circulated prior to the meeting)

	Principles 1			**Principles 2**		
Chapter Name	**Number**	**Pages**	**Chapter Name**	**Number**	**Pages**	**Writer**
Preface	0	2	Preface	0A	2	Leigh
Introduction	1	2	Introduction	1A	2	Leigh
Definitions	2	6	Definitions	2A	6	Leigh
Formulae	3	17	Formulae	3A	?	Leigh
Naming of Substances	4	62	Naming of Substances	4A?	?	?
			Inorganic Nomenclatures	4B?	?	Hartshorn
			Organic Nomenclatures	4C?	?	Favre
			Other Nomenclatures	4D?	?	?
Aspects of Organometallic Nomenclature	5	5	Aspects of Organometallic Nomenclature	5A	?	Hutton
Macromolecular Nomenclature	6	11	Macromolecular Nomenclature	6A	?	Hess
Biochemical Nomenclature	7	10	Biochemical Nomenclature	7A	?	Moss
			InChIs and PINS	7B	?	McNaught
Nomenclature in the making	8	2	Nomenclature in the making	8A	2	?

Index	-	7	Index	-	?	?

Following the August 3-4 meeting, this plan was amended in the following ways.

1. The Chapter 3 A is to be split, and the discussion of stereochemistry moved so as to follow the Chapters on naming. Substances. It is to be expanded to include some discussion of inorganic formalisms (writers Leigh/Hartshorn).
2. The order of sections within 4 is to be changed to organic, inorganic, organometallic.
3. Macromolecular and Biochemical (the latter slightly expanded from the version in Principles 1) to be followed by a brief discussion of other nomenclatures (writer Leigh, perhaps in collaboration with Moss).
4. The index to be constructed by a professional chemist (Hellwich volunteered to do this).
5. The discussion of PINS might eventually be moved to 8A.
6. All contributions to be carefully framed so that only indicative parts of more advanced nomenclature be included along with the basic principles, bearing in mind that the intended audience consists of teachers, lecturers, and students in schools and in the initial years of University study.
7. Writers are encouraged to use flow charts to show how to construct names.
8. Attempts should be made to indicate how chemical structures may be derived from names.
9. Tables should be numbered sequentially and collected together at the end of the volume.
10. Each Chapter should include its own listed references: how these might be treated in the final version was not discussed.
11. Ti ensure the appropriateness of the content, opinions of the May drafts be solicited from organisations such as IUPAC's CCE, practising teachers, and the UK Association for Science Education (approaches to be made by Hartshorn, Hutton, Leigh, and anyone else who has a suitable contact). CCE have already consented to cooperate.
12. Steps should be taken to ensure that the internal IUPAC review of final manuscript should be as short as possible, since the text will rely on approved IUPAC material as sources (this has already been broached informally with ICTNS).

APPENDIX V

Proposal for Revision of Boundaries for Application of Organic PIN Rules and Inorganic PIN Rules

Summary

The alignment project meetings of 2001 and 2002 established draft boundaries within which the organic and inorganic PIN rules could be applied. This proposal from the Inorganic PINs Task Group recommends an adjustment of these boundaries to better reflect the likely expectations of the user communities and to achieve more consistency with the rules that are currently being formulated for the selection of inorganic PINs, and more specifically, with the rules for the selection of central or principal atoms when additive nomenclature will be used for PINs.

The Current Situation

The alignment project meetings laid out draft boundaries that would allow groups working on organic and inorganic PINs to move forward on the projects. According to this agreement, a chemical structure containing an atom from groups 1-12, or 18 should have an inorganic PIN. Any structure containing only atoms from groups 13-17 would have an organic PIN if it contained at least one carbon atom. Otherwise, it would have an inorganic PIN, most likely derived using additive nomenclature. The current proposal for selection of central/principal atoms in such structures identifies particular kinds of atom that will always be treated as central atoms if they are present in the structure.

The resulting classification of atoms is illustrated in Figure 1. Those in black will always be central atoms if they are present and structures containing them will normally be named additively. Those in purple will be central atoms if the structure is named additively, which will either be when there is an atom from groups 1-12, or 18 present, or when there is no carbon present. Those in red will be identified as central atoms on the basis of their connectivity (atoms with the most atoms attached will be treated as central/principal atoms), provided no carbon is present and there are no black or purple atoms. If carbon is present, structures made up of red and purple atoms only will be given an organic PIN.

In the context of central/principal atom choice, the purple atoms have been treated much like black atoms because it is the view of the Inorganic PINs Task Group that in most cases such structures would be treated as inorganic or coordination compounds by the chemical community.

The New Proposal

Given that the black and purple atoms in Figure 1 are all automatic central atom choices if an inorganic PIN is to be used, we believe that we should consider moving the group 12-13 split of the original proposal to be consistent with this differentiation of central atom choice. This placement of a demarcation line is consistent both with our view that a large fraction of structures containing these atoms will be widely identified as inorganic species by the chemical community, and with the classic differentiation that is often made between metals and non-metals even in high school chemistry classes.

The resulting situation is shown in Figure 2. According to this proposal, structures containing any of the black atoms will receive an inorganic PIN, and all such black atoms would be treated as central/principal atoms if the PIN is constructed using additive nomenclature. Structures containing no black atoms would be given organic PINs if they contain carbon, and inorganic PINs if they do not. We believe that this is a simpler overall approach and should be adopted as part of the overall
PINs rules.

1																	18
1 **H**	2											13	14	15	16	17	2 **He**
3 **Li**	4 **Be**											5 **B**	6 **C**	7 **N**	8 **O**	9 **F**	10 **Ne**
11 **Na**	12 **Mg**	3	4	5	6	7	8	9	10	11	12	13 **Al**	14 **Si**	15 **P**	16 **S**	17 **Cl**	18 **Ar**
19 **K**	20 **Ca**	21 **Sc**	22 **Ti**	23 **V**	24 **Cr**	25 **Mn**	26 **Fe**	27 **Co**	28 **Ni**	29 **Cu**	30 **Zn**	31 **Ga**	32 **Ge**	33 **As**	34 **Se**	35 **Br**	36 **Kr**
37 **Rb**	38 **Sr**	39 **Y**	40 **Zr**	41 **Nb**	42 **Mo**	43 **Tc**	44 **Ru**	45 **Rh**	46 **Pd**	47 **Ag**	48 **Cd**	49 **In**	50 **Sn**	51 **Sb**	52 **Te**	53 **I**	54 **Xe**
55 **Cs**	56 **Ba**	*57-71 lanthanoids	72 **Hf**	73 **Ta**	74 **W**	75 **Re**	76 **Os**	77 **Ir**	78 **Pt**	79 **Au**	80 **Hg**	81 **Tl**	82 **Pb**	83 **Bi**	84 **Po**	85 **At**	86 **Rn**
87 **Fr**	88 **Ra**	‡89-103 actinoids	104 **Rf**	105 **Db**	106 **Sg**	107 **Bh**	108 **Hs**	109 **Mt**	110 **Ds**	111 **Rg**							

Figure 1. Classifi cations of elements in relation to use of organic or inorganic PINs and the selection of principal atoms (fr inorganic PINs), based on the boundaries initially agreed at the alignment meetings in 2001-2

1																	18
1 **H**	2											13	14	15	16	17	2 **He**
3 **Li**	4 **Be**											5 **B**	6 **C**	7 **N**	8 **O**	9 **F**	10 **Ne**
11 **Na**	12 **Mg**	3	4	5	6	7	8	9	10	11	12	13 **Al**	14 **Si**	15 **P**	16 **S**	17 **Cl**	18 **Ar**
19 **K**	20 **Ca**	21 **Sc**	22 **Ti**	23 **V**	24 **Cr**	25 **Mn**	26 **Fe**	27 **Co**	28 **Ni**	29 **Cu**	30 **Zn**	31 **Ga**	32 **Ge**	33 **As**	34 **Se**	35 **Br**	36 **Kr**
37 **Rb**	38 **Sr**	39 **Y**	40 **Zr**	41 **Nb**	42 **Mo**	43 **Tc**	44 **Ru**	45 **Rh**	46 **Pd**	47 **Ag**	48 **Cd**	49 **In**	50 **Sn**	51 **Sb**	52 **Te**	53 **I**	54 **Xe**
55 **Cs**	56 **Ba**	*57-71 lanthanoids	72 **Hf**	73 **Ta**	74 **W**	75 **Re**	76 **Os**	77 **Ir**	78 **Pt**	79 **Au**	80 **Hg**	81 **Tl**	82 **Pb**	83 **Bi**	84 **Po**	85 **At**	86 **Rn**
87 **Fr**	88 **Ra**	‡89-103 actinoids	104 **Rf**	105 **Db**	106 **Sg**	107 **Bh**	108 **Hs**	109 **Mt**	110 **Ds**	111 **Rg**							

Figure 2. Classifi cation of elements in relation to use of organic or inorganic PINs based on suggested revised boundaries

APPENDIX VI

Translations of IUPAC Recommendations and Technical Reports into German

Gerrit Schüürmann

Modellierung der Lebensdauer und Abbaubarkeit organischer Verbindungen in Luft, Boden und Wasser
Angew. Chem. **2005**, *117, Nr. 5*, 834 – 845
Original: *Pure Appl. Chem.* **73**, 1331 – 1348 (2001)

Dietmar Schomburg

Nomenklatur der Lignane und Neolignane
Angew. Chem. **2005**, *117, Nr. 15*, 2339 – 2351; **2006**, *118, Nr. 23*, 3983
Original: *Pure Appl. Chem.* **72**, 1493 – 1523 (2000)

Carlo Thilgen

Nomenklatur der Fullerene C_{60}-I_h und C_{70}-$D_{5h(6)}$
Angew. Chem. **2005**, *117, Nr. 31*, 5065 – 5108
Original: *Pure Appl. Chem.* **74**, 629 – 695 (2002)

Hans Schick,* Karl-Heinz Hellwich,* Kathrin-Maria Roy

Überarbeiteter Abschnitt F: Naturstoffe und verwandte Verbindungen
Angew. Chem. **2005**, *117, Nr. 47*, 7985 – 8014; **2006**, *118, Nr. 23*, 3983
Original: *Pure Appl. Chem.* **71**, 587 – 643 (1999); **76**, 1283 – 1292 (2004)

Werner Steck,* Karl Cammann

Harmonisierter Leitfaden für die Validierung von Analysenmethoden durch Einzellaboratorien
Angew. Chem. **2006**, *118, Nr. 12*, 2019 – 2034
Original: *Pure Appl. Chem.* **74**, 835 – 855 (2002)

Karl-Heinz Hellwich*

Phannomenklatur Teil I: Phanstammnamen
Angew. Chem. **2006**, *118, Nr. 23*, 3967 – 3984; **2006**, *118, Nr. 35*, 6032
Original: *Pure Appl. Chem.* **70**, 1513 – 1545 (1998)

Karl-Heinz Hellwich,* Kerstin Ibrom

Phannomenklatur Teil II: Änderung des Hydrierungsgrades und Substitutionsderivate von Phanstammverbindungen
Angew. Chem. **2006**, *118, Nr. 35*, 6023 – 6033
Original: *Pure Appl. Chem.* **74**, 809 – 834 (2002)

Heiko Lueken

Praktische Anleitung zur Messung und Interpretation magnetischer Eigenschaften
Angew. Chem. **2006**, *118, Nr. 47*, 8233 – 8240
Original: *Pure Appl. Chem.* **77**, 497 – 511 (2005)

Ulrich Jonas,* Patrick Theato*

Definitionen von Grundbegriffen mit Bezug zu Polymerreaktionen und zu funktionellen polymeren Materialien
Angew. Chem. **2007**, *119, Nr. 11*, 1955 – 1965
Original: *Pure Appl. Chem.* **76**, 889 – 906 (2004)

Patrick Theato*

Die Terminologie von Polymeren mit ionisierbaren oder ionischen Gruppen und von Polymeren, die Ionen enthalten
Angew. Chem. **2007**, *119, Nr. 23*, 4480 – 4483
Original: *Pure Appl. Chem.* **78**, 2067 – 2074 (2006)

APPENDIX VII

Nomenclature World Wide Web Database – Statistics

Statistics based on log of IP addresses used each day. Total usage to date about 7 240 000. Data on 208 countries recorded so far. Summary data for 1996-2006 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	2006	2007
Total usage	296	650	1476	2786	5515	9813	15360	19105	20392	24617	29261	31481
Search Facility	-	-	-	204	1663	4169	8355	11308	12192	15071	13570	8070
Bibliographic Data	-	61	142	235	325	470	598	655	706	787	826	793
Map of Usage	-	7	8	29	37	58	83	78	107	131	171	169
IUPAC Nomenclature												
Class Names Glossary	138	157	430	693	1039	1504	2178	2492	2836	2944	3210	2737
Atomic Weight	23	48	95	144	310	651	964	1431	1525	1926	2247	2528
Physical Org Chem Glossary	29	36	136	343	751	1089	1796	1934	1782	1714	2008	1840
Periodic Table	-	-	-	17	155	291	475	870	782	999	1198	1413
Stereochemical Glossary	-	32	85	135	231	392	602	694	778	942	1169	1002
Section F (Natural Products)	-	-	-	14	121	321	450	505	583	783	916	845
Medicinal Chemistry Glossary	-	-	56	87	150	316	532	601	636	708	750	676
Bioinorganic Glossary	-	-	61	108	201	391	633	570	523	664	689	522
Fused Ring -	-	64	73	110	198	241	275	299	342	415	402	
Fullerene numbering	-	-	-	-	-	-	-	-	-	118	189	298
Ions and Radicals	-	-	-	-	72	150	196	226	245	278	328	293
Fullerenes -	-	-	-	-	-	69	124	162	232	246	249	
Regular Organic Polymer	-	-	-	-	-	-	-	-	141	236	277	235
Phanes -	-	31	42	56	80	95	135	181	209	231	230	
Hantzsch Widman	12	14	31	46	56	89	116	125	154	195	216	214
Element Name > 100	-	-	-	20	45	78	87	93	147	170	193	170
von Baeyer -	-	-	29	61	106	130	118	133	164	167	156	
Spiro -		-	26	47	90	114	115	137	163	172	155	
Section H (Isotopic Label)	-	-	26	34	46	73	90	93	112	154	162	123
Numerical Term	-	18	27	35	54	99	150	189	238	325	238	122
Delta Convention	8	9	19	30	54	82	110	106	121	130	133	114
Lambda Convention	6	8	17	28	40	60	76	74	85	101	110	92
Phane II -	-	-	-	-	-	-	59	68	86	88	89	
Guide Errata -	-	-	20	21	25	32	47	53	68	68	54	
IUPAC/IUBMB Nomenclature												
Amino Acids & Peptides	31	62	135	186	359	670	1072	1366	1594	1918	2286	2347
Carbohydrates	46	72	144	237	453	835	1156	1444	1266	1238	1519	1518
Steroids 12	21	87	93	396	811	1213	1460	835	555	755	913	
Folic acid -	-	-	60	58	210	208	304	284	293	302	391	
Nucleic Acid Abbreviations	-	-	-	45	77	136	202	241	256	325	348	373
Lipids -	-	-	29	70	132	198	232	252	302	334	373	

	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006	2007
Tetrapyrroles-	-	-	-	-	124	221	227	240	335	385	369	
Vitamin D -	-	-	-	47	69	125	209	385	348	342	317	
Vitamin B-6 -	-	-	34	95	155	267	466	306	302	333	233	
Lignans and Neolignans	-	-	-	-	-	71	123	137	170	237	235	227
Glycoproteins	-	-	20	32	71	134	172	187	185	232	250	221
Tocopherol -	-	21	33	48	80	150	274	232	260	233	205	
Cyclitols -	-	21	51	72	113	174	178	177	207	194	201	
Polypeptide Conformation	-	8	14	34	61	111	173	191	182	202	210	200
Carotenoids -	-	-	-	46	84	128	148	167	199	208	199	
Glycolipids -	-	15	35	65	91	137	171	213	234	230	192	
Vitamin B-12	-	-	-	49	69	146	266	315	227	164	197	162
Polynucleotide Conformation	-	7	15	27	44	68	92	103	124	164	170	157
Polysaccharide Conformation	-	8	14	26	49	82	134	153	155	162	161	144
Retinoids -	-	-	-	35	71	99	126	140	136	143	127	
Biochemical Phosphorus	-	-	-	-	62	103	151	147	133	139	138	125
Quinones with Isoprenoid Chain	-	-	-	-	-	47	90	105	116	162	146	120
Prenols -	-	-	19	33	55	77	84	108	127	122	105	
Polymerised Peptides	-	-	-	-	34	56	91	97	109	118	120	110
Both Biochemical Committees												
Committees' Homepage	18	38	65	123	268	423	653	801	1015	1218	881	410
Newsletter -	-	25	59	145	304	456	446	490	659	836	864	
IUBMB Nomenclature												
Enzymes 16	54	124	320	1086	2088	3560	4260	5459	8837	12508	13172	
EC 1 -	-	-	35	241	487	922	1091	1497	2721	4259	4161	
EC 2 -	-	-	-	180	438	769	900	1242	2358	3510	3330	
EC 3 -	-	-	-	165	427	947	1054	1496	2333	3720	3795	
EC 4 -	-	-	-	90	223	410	423	635	1215	1547	1518	
EC 5 -	-	-	-	64	164	294	322	441	720	826	849	
EC 6 -	-	-	-	46	138	239	261	374	674	770	814	
reaction -	-	-	-	48	119	381	650	1089	2295	3134	3121	
newenz -	-	-	-	53	60	75	71	86	84	90	90	
Enzyme Kinetics	-	-	16	61	152	249	365	441	547	687	926	944
Biochemical Thermodynamics	-	-	22	40	66	107	132	148	170	224	284	293
Incomplete Nuc. Acid Sequence	-	9	20	31	50	75	103	137	205	293	304	288
Membrane Transport Proteins	-	-	-	-	-	-	93	157	188	287	325	252
Electron Transport Proteins	-	-	-	-	58	107	163	165	168	225	242	214
Peptide Hormones	-	-	-	-	32	51	80	101	115	130	145	136
Isoenzymes -	-	14	28	68	106	124	123	135	159	156	130	
myo-inositol -	-	11	23	43	74	125	125	113	139	118	129	
Multienzymes	-	-	10	13	18	25	37	36	43	52	51	54
Branched Chain Nucleic Acids	-	3	6	10	40	63	115	107	89	110	78	46
Translation Factors	-	-	-	-	11	18	34	37	42	41	32	29