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

Ottawa, Canada, August 9-10, 2003

Members Present: Dr Stephen Heller (Aug 9, only), Prof Michael Hess (in part), Prof Herbert Kaesz, Prof G. Jeffrey Leigh, Dr Alan McNaught (President), Dr Gerard Moss, Dr Warren Powell (Secretary), Dr William Town.

Members Elected for 2004 Present: Dr Ture Damhus (Aug 10, only), Prof Richard Hartshorn, Prof Jaroslav Kahovec, Prof József Nyitrai, Dr Matthew Toussant (Aug 9, only), Prof Andrey Yerin

Representatives from other IUPAC bodies present: Prof Richard Cammack (JCBN)

National representatives Present: Prof Jiasong He (in part), Prof Bernado Herold

Members Absent: Dr. Michael Dennis, Prof Dr Alexander Lawson, Dr. Antony Williams

The third meeting of the Division Committee of the IUPAC Division of Chemical Nomenclature and Structure Representation held at the University of Ottawa in Ottawa, Canada, was convened by President McNaught at 9:00 a.m. on Saturday, August 9, 2003.

1.0 President McNaught welcomed the members to this meeting and offered a special welcome to the new members elected for 2004 and to Prof Richard Cammack as a new ex officio member (as Chairman of JCBN). He also noted that Dr Michael Dennis, Prof Alexander Lawson, and Dr. Antony Williams would be unable to be with us. Each of the attendees introduced himself and provided background information. Housekeeping details regarding breaks and lunch were announced.

2.0 The agenda as circulated was approved with the addition of a report from Dr Moss on the activity on his website.

3.0 The minutes of the Division Committee Meeting in Boston, Massachusetts, USA, on August 18, 2002 as posted at
http://www.rsc.org/IUPAC8/attachments/DivisionCommitteeMinutesBostonFinal.doc
http://www.rsc.org/IUPAC8/attachments/DivisionCommitteeMinutesBostonFinal.pdf
were approved with no corrections.

4.0 Matters arising from the minutes

4.1 Following the Bureau meeting in September 2002, new model Division Rules and Terms of Reference were prepared by the Secretary General. The Division Rules and Terms of Reference for Division VIII based on these new model rules are posted at
http://www.rsc.org/IUPAC8/attachments/DivisionVIIIRules2003.rtf
http://www.rsc.org/IUPAC8/attachments/DivisionVIIIRules2003.pdf
Currently, the electorate established by the IUPAC Secretariat for elections of Titular Members and Associate Members consists of the Titular Members, Associate

Members, National Representatives, Chairpersons of Division Task Groups and 'outside' members of the Nominating Committee. Several Divisions want a broader electorate. After discussion, it was agreed to go back to the Bureau to expand the electorate, in our case, to include members of the Advisory Subcommittee.

5.0. IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN)

5.1 Reconstitution of JCBN. Since JCBN was not a part of the general restructuring of IUPAC that took place in Brisbane (2002), a proposal prepared by A. McNaught in consultation with R. Cammack (Chairman of JCBN and NC-IUBMB) was presented to the Bureau at its meeting in September, 2002. It was described in an attachment to the Boston Division VIII Committee minutes. Further discussions and the resulting recommendations are documented in a report by A. McNaught which can be seen at

http://www.rsc.org/IUPAC8/attachments/JCBNReconst-DivVIII03.rtf
http://www.rsc.org/IUPAC8/attachments/JCBNReconst-DivVIII03.pdf .

G. P. Moss, R. Cammack, W. Powell, and A. McNaught met in Ottawa to discuss future membership for JCBN to submit to the Bureau and to IUBMB for approval. The following was to be proposed:

	Titular Members	Associate Members
JCBN	Prof. R. Cammack (IUBMB) (Chairman) Prof. J. F. G. Vliegenthart (IUBMB) Dr. S. Boyce (IUPAC) (Secretary) Dr. G. P. Moss (IUPAC)	Prof. D. Horton Dr. M. A. Chester Dr. A. Cornish-Bowden Prof. D. Schomberg Dr. T. Kazic Prof. F Vella.

R. Cammack was to approach Vliegenthart and Vella to confirm that they were willing to serve.

5.2. Report of the meeting, Dublin, May 2003. R. Cammack and G. P. Moss summarized the meeting of the Nomenclature Committee of IUBMB (NC-IUBMB) and IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN) held in Dublin in May, 2003. The minutes of the meeting are given in Appendix I.

R. Cammack is to prepare a project proposal for the next set of recommendations for carbohydrate nomenclature, on behalf of D. Horton. It will update the 1996 Recommendations. The target date for publication will be 2006.

JCBN is keeping a close eye on the development of databases at the European Bioinformatics Institute (EBI); there should be a closer link with IUPAC names.

The enzyme list is now updated only on the Web. No supplements to the published Enzyme list are planned. Like NC-IUBMB, CAS classifies enzymes based on activity. CAS has a concordance containing some 250,000 entries. Cooperation between NC-IUBMB and CAS should be further developed so that new listings in CAS can be referred to NC-IUBMB for assignment of E.C. numbers.

News items are needed for the next Newsletter under preparation by R. Cammack. It could include new enzymes under review.

5.3. B. Herold will check the ICTNS files concerning the status of a document on the nomenclature of cyclic peptides. G. Moss will submit the current draft for posting on the Webboard, followed by whatever review is required.

6.0 Division VIII Publications:

6.1 An Article on 'Phane Nomenclature' by Henri Favre and Warren Powell was published in "Cyclophane Chemistry for the 21st Century" (Research Signpost, 2002). Reprints are available from W. Powell.

6.2 An article "Unique Labels for Compounds" describing the IChI project by Michael Freemantle appeared in *Chemical & Engineering News*. It can be found at http://pubs.acs.org/cen/today/nov26.html .

6.3. A new article about IChI by A. D. McNaught will appear in *Chemistry in Britain* (to become *Chemistry World* in 2004) when the next version of the program is ready.

7.0 Division VIII projects

7.1 IUPAC Chemical Identifier. A status report was given by S. Heller.

The most important feature that distinguishes this system from others is "layering", i.e., separation of various levels of structural information, such as molecular formula, connectivity information, stereochemical information, isotopic labeling, tautomers, etc. into 'layers'. This approach enables chemists to represent compounds at a level of detail of their choice. If there is insufficient information to generate a layer, that layer is left out of the identifier.

For searching it will be up to chemical software manufacturers and user organizations to develop software, according to individual strategies and goals.

A project meeting will be held in Washington, D. C. in November, 2003.

The present version of the software deals with organic covalent structures. Extension to organometallic and coordination structures and polymers is planned. It is hoped to establish a contact with Gmelin to obtain input on inorganic compounds. So far, that has not materialized.

7.2. Preferred IUPAC Names for Organic Compounds.

A complete draft of the new edition of the 'Blue Book' which contains the rules necessary for deriving preferred IUPAC names for organic compounds has been finished. It consists of nearly 1200 manuscript pages (single spaced) and has been posted on the Division VIII Webboard in some twenty different files for review by Division VIII Committee members and members of the Division VIII Advisory Subcommittee. Comments received before August 6 on Chapters 1-5 were reviewed at the meeting of the Task Group on August 6-7. Comments on the rest of the chapters and other comments received by November 15 will be reviewed at another Task Group meeting in Washington, D. C. on November 18-19.

Chapter 10 of the new 'Blue Book' deals extensively with natural products and related compounds. As such it relies extensively on the Section F of the 1979 'Blue Book' and its revision published in 1999. Subsequent to the publication of the

Revised Section F, a number of errors and modifications have been noted. An 'Errata' notice was prepared by G. P. Moss following review by a group of interested persons in Boston, 2002. Since then, further changes had been proposed, and A. McNaught and G. P. Moss would meet (in London) to consider all of these and prepare a new 'Errata' notice for circulation to those who met in Boston. Agreed changes to the Revised Section F would be incorporated into the Web version and the new 'Errata' notice published in PAC. These corrections and agreed changes will be incorporated into Chapter 10 of the new 'Blue Book'.

It is planned to have a revised draft of the new Blue Book ready for public review by early next year. It will be posted on the IUPAC Web site. The final publication is expected by the end of 2004.

7.3 Revision of the "Nomenclature of Inorganic Chemistry" (Red Book). The revised 'Red Book' has been posted on the Division VIII Webboard for review by Division VIII Committee members and members of the Division VIII Advisory Subcommittee. It is planned to have a final draft ready for posting on the IUPAC Web site for public review by November. Final publication is expected by the end of 2004.

7.4 Fullerenes, Part II. A complete draft of the procedures for numbering fullerenes other than the C_{60}-I_h and C_{70}-$D_{5h(6)}$ fullerenes and their derivatives [published in *Pure Appl. Chem.* Vol. 74, No. 4, pp. 629-695 (2002)] prepared by F. Cozzi was reviewed at a meeting of the Task Group in Ottawa, August 7-8, 2003. Nearly fifty fullerenes belonging to a variety of symmetry point groups have been successfully numbered using the rules developed by the Task Group. Corrections and suggested modifications to the draft were to be incorporated by F. Cozzi. A goal of this project was to provide numbering for all fullerenes with known structures. The list of these fullerenes was updated and those not included in the current draft were to be numbered. A finished draft is expected to be posted on the Division VIII Webboard by the end of the year.

7.5 Rotaxanes. A project on nomenclature of macromolecular rotaxanes originated in the former Commission on Macromolecular Nomenclature under the leadership of E. Wilks was transferred to Division VIII. It has been split into two parts, one dealing with molecular rotaxanes (earlier termed 'discrete' rotaxanes; the term 'discrete' has now been dropped) and the other with macromolecular rotaxanes. A first draft of the former has been prepared and is posted on the Division VIII Webboard for comment. The new Task Group Chairman is A. Yerin.

7.6 Macromolecular projects

7.6.1 Macromolecular rotaxanes. E. Wilks has asked to end his responsibility as coordinator of this project as well as the project on molecular rotaxanes (see 7.5). Since it is desirable for publications on both rotaxane projects to appear at the same time and the macromolecular recommendations depend to some extent on the content of the molecular rotaxane document (see 7.5), the former has been put on hold until more progress has been made with the latter. The Task Group leader will be determined in 2004. However, the

latest draft of the macromolecular project was reviewed and E. Wilks agreed to provide a revised draft.

7.6.2 Dendritic and hyperbranched polymers. After discussions at the Beijing meeting a new draft was prepared, circulated among the members of the working party, comments submitted, and a new version prepared which was the subject of the discussions in Ottawa. As a result, the title was modified to 'Nomenclature and Terminology for Organic Dendrimer, Hyperbranched Oligomeric, and Polymer Molecules'. Some particular terms were revised. Harmonization with other existing documents and with documents currently in preparation has yet to be performed. A new draft will be prepared on the basis of these discussions. The document was scheduled to be finished by the end of the year 2003; however, an extension of one year is recommended and the document is expected to be ready for public review towards the end of the year 2004. A corresponding project extension will be submitted. J. Kahovec continues as the Task Group leader.

7.6.3 Macromolecules with cyclic structures. The Task Group Chairman is W. Mormann. K-H. Hellwich has joined the task group. Two drafts, based on input from both Divisions IV and VIII had been prepared following the meetings in Beijing. A fundamental problem concerning seniority in cyclic heteroatom systems was solved. It is hoped that the next version will soon be ready to go to external experts so that a final draft can go for public review in 2004. The project will require a one year extension for which the appropriate requests are being made.

7.6.4 Chemically modified polymers. Some fundamental questions about the project which had surfaced after the Beijing meeting were discussed and solved so that on the basis of the Ottawa discussions a new draft can be prepared. The project is now titled 'Nomenclature and Graphic Representation for Chemically Modified Polymers. The present project coordinator, E. Wilks, resigned from this position and T. Kitayama from Division IV was named the new Task Group chairman. He will provide a revision and a new draft. It is assumed that the project will require about two more years for its finalization and a corresponding project extension will be submitted. E. Wilks will continue to participate in the working party.

7.6.5 A new project called 'Source-Based Nomenclature on Copolymers' (T. Kitayama and I. Mita) was introduced. It will be expanded to include homopolymers and given the title 'Source-Based Nomenclature of Single-Strand Organic polymers'. Because of its nomenclature character it will become a Division VIII project run in collaboration with Division IV. A project application form will be submitted by the end of September and the first draft is scheduled for completion by the end of May 2004. The task group will consist of T. Kitayama, I. Mita (coordinator), P. Kratochvil, R. Stepto, S. Penczek, A. Fradet, E. Wilks, J. Vohlidal, M. Hess, C. Ober and K. Thurlow (Chairman of ISO/TC61 Plastics, SC1 Terminology). There is the possibility that there will be three more members.

8.0. Division VIII Scoping Exercises

8.1 Stereochemistry. In an attempt to generate projects for future work, a scoping exercise to detect problems in stereochemical nomenclature was established at the Division Committee meeting in Cambridge, January, 2002. Comments on a project proposal prepared following the Division Committee meeting in Boston, August, 2002, indicated that the topic was too broad and needed to be broken down into smaller chunks. A core group consisting of R. Hartshorn, G. P. Moss, and K-H. Hellwich met in Ottawa on August 8 to develop further proposals. It was suggested that J. Wisniewski be involved because of his experience in using the CIP system for designating configuration at tetrahedral carbon atoms.

8.2 Structure representation. In an attempt to generate projects for future work, a scoping exercise to study graphical representation of chemical structures was established at the Division Committee meeting in Cambridge, January, 2002. During the past 16 months J. Brecher and his collaborators (P. Giles, H. Gottlieb, P. Murray-Rust, B. Ramsay, A. Smith, S. Stein, K. Taylor, W. Town, A. Williams and A. Yerin) have been exploring requirements for IUPAC guidelines on representation of chemical structures. They produced the attached report (Appendix II), web-linked to extensive draft guidelines. Clearly, there are a number of projects to be studied. W. Town agreed to develop specific projects on this subject.

The one-wedge convention for graphical representation of stereoformulas, a paper reviewed earlier by the IUPAC Commission on Nomenclature of Organic Chemistry, has been published in *Molecules*. This topic is still open in ICTNS and ICTNS should be informed formally that this matter has been absorbed into a Division VIII project on structure drawing.

9.0 Inorganic nomenclature. A working group to develop inorganic nomenclature projects recommended at the Boston Division Committee meeting met in Cambridge in April, 2003. The minutes of this meeting can be seen at

http://www.rsc.org/IUPAC8/attachments/DivVIIIinorgWP03.rtf
http://www.rsc.org/IUPAC8/attachments/DivVIIIinorgWP03.pdf

Some 12 potential projects were identified. A proposal to choose descriptors for complexes with seven coordination sites has been submitted. A project involving structure representation in formulas could be absorbed into the structure representation project noted above. In addition, a proposal on nomenclature of borophosphates has been submitted.

H. Kaesz raised questions about the future of this working group. Should it become a Subcommittee of the Division VIII Committee? Should it remain as an 'ad-hoc' committee. It was felt that the group should continue to coordinate the development of inorganic nomenclature projects on an 'ad-hoc' basis, and G. J. Leigh would consider planning a further meeting. Exactly how the group should be titled was not determined.

The use of the term 'ligand' was discussed. It is used differently in biochemical nomenclature, coordination nomenclature, and in stereochemical nomenclature. This question probably should be brought into the open by publication as a note, included in a Newsletter, or just posted on the Division VIII Webboard.

10.0 Committee on Printed and Electronic Publications (CPEP). S. Heller noted the following from CPEP:

(1) JCAMP (Joint Committee on Atomic and Molecular Physical Data) activities have been transferred to a CPEP Subcommittee on Spectroscopic Data Standards.

(2) CPEP is moving toward spending most of its effort on strategy rather than on details of book publishing books and journals.

(3) The XML project is moving along very well. The Gold Book is the first to be processed and the Green Book will follow when the new revision is available. There is close communication and interaction with Chemical Markup Language (CML: P. Murray-Rust and H. Rzepa).

(4) There will be an XML/IChI meeting at NIST on November 12-14, 2003.

11.0 Future Division activities. Proposals for the following projects from the report of the 'ad-hoc' inorganic nomenclature committee should be developed as soon as possible.

(1) Preferred names for 'inorganic', i.e., noncarbon containing compounds; for Groups 13-17 these are called preselected names in the organic preferred names book. A list of problems encountered during the revision of the Red Book should be prepared.

(2) Organometallic compounds. i.e., derivatives of the metallic elements of Groups 13-16 with at least one direct carbon bond to the central atom. Presumably, this effort would include elements in Groups 1 and 2. But would it include the elements of Group 18?

(3) Generalized cluster nomenclature. An earlier paper by T. Sloan, W. Powell, and D. Coucovanis should be taken into consideration.

(4) Boron nomenclature.

12.0. Publicity.

12.1 Suggestions for publicity made at the Division VIII Open Meeting, August 8, as follows were reviewed.

(1) Publicize at international meetings and conferences

(2) Periodic, such as once a year, mailings to journals

(3) Make appearances at IUPAC sponsored conferences.

(4) Put on workshops or produce audio tapes (like the ACS audio tape program).

(5) Offer publishers a 'nomenclature IUPAC approved' stamp for papers and textbooks.

(6) Publication of the new Blue Book, Red Book, and Purple Book provides an opportunity to alert journal editors, patent lawyers, and pharmaceutical firms to the existence of IUPAC recommendations.

12.2. Other suggestions included the following

(1) Produce an annual Division Newsletter to send to journal editors. Include a summary of activities and short announcements of upcoming projects.

(2) Produce a one sheet summary of publications and where to find them to circulate at conferences, National Adhering Organizations, and journal editors.

(3) From his work on the nomenclature website G. P. Moss had accumulated some 1200-1300 e-mail addresses that could be used as a mailing list of persons interested in nomenclature.

(4) Develop tutorials and prepare short publications, such as the Phane publication noted earlier (6.1), for circulation.

(5) Prepare a revised edition of "Principles of Chemical Nomenclature".

(6) In any publicity material, some complex documents such as the Revised Red Book and Blue Book, would need explanatory material.

H. D. Kaesz agreed to take responsibility for developing and coordinating Division VIII publicity activities. He would draw up a publicity plan and circulate to Committee Members for comment. This would include a suggested list of items for the first Division Newsletter.

13.0 Division Membership for 2004-2005.

13.1 Titular Members 2004-2005. Four current memberships expire at the end of this year (M. Dennis, M. Hess, G. J. Leigh, and A. Williams). Five Titular Memberships continue until 2005 (A. D. McNaught, W. H. Powell, H. D. Kaesz, G. P. Moss, A. Williams). The Division Committee may have ten Titular Members. Thus, the following new Titular Members had been elected by mail ballot, each for four year terms:

T. Damhus (2004-2007)
R. Hartshorn (2004-2007)
J. Kahovec (2004-2007)
J. Nyitrai (2004-2007)
A. Yerin (2004-2007)

13.2 In addition, it was necessary to elect a Vice-president, who will automatically succeed to President in 2006. There were two candidates nominated and who accepted to stand for election, G. P. Moss and H. D. Kaesz. G. P. Moss was elected by show of hands.

13.3 The complete list of Titular Members of the Division Committee starting in 2004 is as follows:

A. D. McNaught (2002-2005) (President)
G. P. Moss (2002-2005) (Vice-president)
W. H. Powell (2002-2005) (Secretary)
H. D. Kaesz (2002-2005)
A. Williams (2002-2005)

T. Damhus (2004-2007)
R. Hartshorn (2004-2007)
J. Kahovec (2004-2007)
J. Nyitrai (2004-2007)
A. Yerin (2004-2007)

13.4 Associate Members 2004-2005. The Division Committee presently has three Associate Members whose terms all expire at the end of 2003. We are entitled to have six Associate Members. It had been agreed by e-mail to appoint the following as Associate Members for 2004-2005:

G. Leigh
M. Toussant
J. Brecher
S. Heller
M. Hess (replacing E. Wilks, who was selected but declined to serve)
S. Lawson

R. Cammack remains an ex officio member as Chairman of JCBN.

13.5 National Representatives 2004-2005. The Division Committee can have six National Representatives, which must be reviewed every two years. We have six at the present time, three of which have shown some interest in the work of the Division. There have been six other nominations. Biographies of all will be circulated and then selection will be made via e-mail ballot.

It had been suggested that there be a 'panel of National Representatives' consisting of a representative from each interested country of which six would be on the Division Committee. This 'panel' would be like our Advisory Subcommittee. This suggestion would be considered at the forthcoming Council meeting.

13.6 Advisory Subcommittee 2004-2005. The present advisory Subcommittee Members are given in

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

and in Appendix III. It was agreed to keep those existing members who wish to remain and add as new members persons who get involved with projects. Dr. Carlo Thilgen, a member of the Fullerene II task group, has indicated that he would like to become a member.

14.0. Division Web Board. The Division Webboard seemed to be working satisfactorily, except for the following observations.

(1) The e-mail alert should contain a copy of the posted message with a direct link to the new file, and

(2) everyone should be alerted to all new additions to the Webboard.

It was also noted that you must 'mark as read' and then 'log-off' to remove 'new' markings from your listing.

15.0 Other Business.

15.1 Activity for the web site maintained by G. P. Moss (not the IUPAC web site) is given as Appendix IV. It was emphasized that this site does not include polymer or inorganic documents. Integration with the IUPAC web site is needed. Ideally, all IUPAC documents should be at one web site. A McNaught will talk with the Publications Committee about integration of the IUPAC web site with the site maintained by G. P. Moss.

15.2. W. Powell was urged to make the necessary adjustments to the document comparing names of derivatives of fused ring systems formed by using nondetachable hydro prefixes, 'added hydrogen' as used by CAS, and 'indicated hydrogen' as used by Beilstein in order that it can be placed on the Webboard in preparation for its publication as a IUPAC Technical Report.

15.3. Contacts with other Divisions with an interest in nomenclature should be maintained. H. Kaesz is an Associate Member of Division II; W. Powell is an Associate Member of Division III; M. Hess is a Titular Member of Division IV and a Task Group Leader; J. Kahovec is an Associate Member of Division IV and a Task Group Leader. Thus, at present, our contacts with other Divisions are good.

Each Division should be contacted requesting information on current or potential problems on terminology.

15.4. A project about PINs for polymers should be considered soon.

15.5. In multilingual dictionaries, non-English names are not the business of IUPAC. However, the English names are often inconsistent and need editing. Could IUPAC sell its services to European publishers for editing English names?

16.0 Next meeting. J. Nyitrai has agreed to arrange the next meeting (2004) of the Division VIII Committee in Budapest. It will most likely be in the latter part of August and the exact dates will depend on the dates for the Fall ACS Meeting.

The meeting was adjourned at noon on August 10.

Respectively submitted.

Warren H. Powell (Secretary)
October 17, 2003

Appendix I

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

Annual NC-IUBMB and JCBN meeting

Bewley's Hotel, Ballsbridge, Dublin, May 3-4 2003

Attendees:

NC-IUBMB and JCBN

Richard Cammack, Chairman (London, UK)
Derek Horton (Washington, DC, USA)
Arnost Kotyk (Prague, Czech Republic)
Keith Tipton (Dublin, Ireland)

NC-IUBMB

Charles Cantor (San Diego, CA, USA)
Gerard Moss (London, UK)

JCBN

Sinéad Boyce, Secretary (Dublin, Ireland)
Keith Elliott (Manchester, UK)
Minoru Kanehisa (Kyoto, Japan)
Nathan Sharon (Rehovoth, Israel)

Others

Rolf Apweiler (Hinxton, UK)	Associate Member of NC-IUBMB
Hal Dixon (Cambridge, UK)	Associate Member of NC-IUBMB
Toni Kazic (Missouri, USA)	Associate Member of NC-IUBMB
Alan McNaught (RSC, Cambridge, UK)	Associate Member of NC-IUBMB
Michael Darsow (Hinxton, UK)	Observer
Kirill Degtyarenko (Hinxton, UK)	Observer
Astrid Fleischmann (Hinxton, UK)	Observer
Andrew McDonald (Dublin, Ireland)	Observer
Tony Merry (Oxford Glycobiology Institute, UK)	Observer
Donald Nicholson (Leeds, UK)	Observer
Hester Wain (HUGO, London, UK)	Observer

1. Welcome and Apologies

The meeting began at 10 am on Saturday 3 May. Cammack, as Chairman, welcomed everyone to the meeting and thanked Tipton and Boyce for making the arrangements. Apologies from Alan Barrett, Helen Berman, Alan Chester, Athel Cornish-Bowden and Dietmar Schomburg were noted.

2. Approval of Agenda

The Agenda was passed as approved.

3. Minutes of the Köln Meeting, May 2002

Minutes of the Köln meeting were approved with no amendment.

4. Matters Arising

Kotyk pointed out that although Kazic's appointment as an associate member of NC-IUBMB was approved at the 2002 meeting, she was not on the list of Committee members. Moss agreed to make the relevant change to the website (http://www.chem.qmul.ac.uk/iubmb/nomenclature/membr.html). **(Action: Moss)**

5. Chairman's Report (Cammack)

Cammack reported that he has taken steps to increase the publicity that the Committees receive. He presented a poster on redox enzymes at the Harden Conference on Electron-Transfer Enzymes that was held at Ambleside, 2002. He reported that he will present a poster at the Toronto Congress, where he will be meeting with the IUBMB Congress. He also reported that a new Newsletter is imminent and this will be placed on Moss' website. Kotyk reported that an article he sent to Sharon for inclusion in the Newsletter has been mislaid so he will resend it to Cammack. Cammack informed the Committees that the Nomenclature Committee of IUBMB is entitled to publish short articles on nomenclature in TiBS, BAMBEd (Biochemistry and Molecular Biology Education) and IUBMB journals.

Cammack stressed the need to get new members of the scientific community involved in nomenclature issues and pointed out that the activities of the Committees are based on the work of dedicated members who produce nomenclature. Tipton asked that the offer by Hans Vliegenthart to provide assistance to the Committees on nomenclature matters be recorded in the Minutes. Moss indicated that Vliegenthart's assistance in the area of carbohydrate enzymes would be most welcome. Cammack said that he was disconcerted by the lack of response to requests for comment on circulars that he had distributed. Dixon said that more explicit indications should be given so that members of the Committees are encouraged to respond even if they have nothing to report. **(Action: Kotyk)**

5.1 Treasurer's report (Elliott)

According to Elliott's records, spending by the Committees over the past year was very low: $2000 from IUPAC and $1000 from IUBMB, but he pointed out that this may not reflect the true state of the Committees' finances as not all of those who claimed expenses sent him notification of the amounts that they claimed. All those paid by IUBMB who claim expenses must send a copy of their claim to Elliott as well as to the treasurer of the IUBMB (Brian Beechey). Cammack spoke to Beechey, who agreed to recommend that the IUBMB continued its funding of the Committees at the same basic level as provided in 2001, but increased slightly to take account of inflation. **(Action: all Committee members claiming expenses)**

6 & 7. Membership and Future of the Committees

This item is related to reorganization of IUPAC and IUBMB. According to documents provided by McNaught and distributed with the Agenda, the JCBN will have fewer titular members and this will have to be implemented by the end of 2003 as the new constitution will take effect from January 1 2004. At present, there are four members of the Committees who are JCBN members only (i.e. not joint NC-IUBMB—JCBN members), namely Boyce, Elliott, Kanehisa and Sharon. In future, JCBN will support only two titular members (one being the Secretary), although up to eight associate members can be appointed. Dixon suggested that two members from the JCBN become titular members of NC-IUBMB instead. This would solve the problem without resulting in any changes to funding, as IUBMB already funds these members. Cammack will draft a proposal.

Kotyk reported that he is retiring as a full member of NC-IUBMB—JCBN although he said that he would still be willing to contribute to the work of the Committees as an associate member. His resignation was accepted with regret by Cammack, who thanked him for his contribution to the work of the Committees. Kotyk asked that he be replaced by someone from the field of membrane proteins and said that he could put forward two or three names. A discussion ensued on mechanisms for attracting new members to the Committees and on the areas of expertise that were required. It was decided that this should be discussed by McNaught and Cammack at a later date.

Elliott indicated that he must step down as a full member of JCBN due to a change in his academic role

although he said that he would be happy to remain associated with the Committees. Sharon indicated that he may retire from the Committees. Horton also indicated that he would be willing to step down from his position if a younger carbohydrate expert could replace him, although he wants to complete the revision of the carbohydrate document before so doing.

The new JCBN Constitution places emphasis on funding for specific projects. Moss pointed out that conjugates are widely used but current names often omit important parts of the molecule. He outlined a need for conjugate nomenclature and said that he would put this forward as a possible project. **(Action: Cammack; McNaught; Moss)**

8. Information on Nomenclature Databases and Related Activities

8.1 Progress on the BioBabel Project (Apweiler, Darsow, Degtyarenko and Fleischmann)

This EU-funded project began on November 1 2001 and will run until October 31 2004. The initial stage of the project, i.e., to develop a database to hold the enzyme nomenclature data is almost complete. The next step is to include the data from Bairoch's ENZYME database and to ensure that, for common data, these data are consistent with the NC-IUBMB-approved data in the Enzyme List. The database is still at the production stage but it is hoped to produce a public version in the near future. The production database can be viewed at http://www.ebi.ac.uk/~mdarsow/cgi-bin/intenz-curation/intenz-dev/intenz/index.jsp. Degtyarenko also informed the Committees about chEBI, another part of the project that aims to provide a standard for biochemical compounds that should be used in databases. McNaught recommended that Degtyarenko liaise with the IUPAC Committee that is creating an XML Chemical Ontology so that he can avoid duplication of effort.

8.2 Kazic's Databases (Kazic)

Kazic informed the Committees that she has bought some domain names, e.g. http://www.biochem.org, which are freely available for use by the Committees. Her databases, (Agora, BND, END, Klotho, Moirai and Glossa) can be accessed from www.biocheminfo.org. BND contains terms drawn from reaction equations in the Enzyme List, which can be used to serve queries against END and the Agora. Version 2.0 of END was released in March 2003 (July 2001 nomenclature) and contains improvements in small-molecule nomenclature. v2.1 will have additional searches (e.g. of PubMed), v2.2 will have all current supplements and v2.3 will correct errata. Her group are currently working on the Agora interface (http://sthenias.cecs.missouri.edu/test_agora/).
49*2

Kazic also indicated that they have a lot more terms to add to their small-molecules database. They can associate any synonym with any primary term, but would like help in assigning primary terms. Cammack asked how terms including a Greek letter can be searched for. Kazic said that the term would have to be spelt out (e.g. 'gamma' for 'γ'). As END is designed for direct user input of draft enzyme entries, Kazic said that they propose to select two reviewers, in addition to the arbiter, who is an expert in the area, but details of reviewer selection etc. have not been decided upon. McNaught asked what the users' motivation would be for adding information. Kazic said that members of the scientific community with interests in particular areas would like to make sure that information in their area is correct. Enzyme data will be sent to the Trinity group for final adjudication and they will use curators for other types of data. Sharon suggested that instructions to authors should include a link to Kazic's site and indicate that users could find it useful. Tipton said that it should be advertised in TiBS.

8.3 Update on KEGG (Kanehisa)

In KEGG (http://www.genome.ad.jp/kegg/kegg2.html), there are many types of data option. Kanehisa and coworkers have been trying to standardize different types of objects using XML (e.g. in KEGG metabolic pathways). An object is represented as a graph with nodes and edges. This can be viewed as a graph of chemical compounds or as a graph of enzymes or enzyme genes. XML represents both types of information. Node information is concerned with enzymes, whereas edges represent chemical compounds. KEGG has different chemical graph objects in the LIGAND database. Currently, they are adding glycan structure information. Chemical information is converted into KCF (Kegg Chemical Format structure). This format gives coordinates for projection in the plane. For example, carbon can be classified

into 15-20 different types, depending on its environment. Users can use a graph-based comparison method to enter a compound and search for results in a database. The search interface is based on a vector.
Kanehisa also mentioned the KEGG Glycan Database (due for release July 2003), which will have methods to compare structures and to browse chemical structures within the database.
Dixon paid tribute to Kanehisa on the accomplishment of KEGG.

8.4 Nicholson Maps and Minimaps (Nicholson)
This was discussed under Item 15.2.

8.5 Update on the Enzyme-List Website (Moss)
Moss provided statistics on the usage of his site in general and, more specifically, with regard to the various categories of information available.

8.6 Update on Hugo (Wain)
Wain gave a presentation on the activities of the HUGO Gene Nomenclature Committee (http://www.gene.ucl.ac.uk/hugo/), who assign and approve gene symbols. She indicated that they provide guidelines on the web and gave information on their naming criteria, resources and chromosome projects. She also talked about their virtual workshops, which they find useful in terms of recruiting members of the scientific community to assist in the task of identifying new genes in the human sequence (see http://www.gene.ucl.ac.uk/nomenclature/workshop/virtual.html). Wain also said that in order to publicize the activities of HUGO, they encourage those publishing papers to indicate that they have used HUGO-approved gene symbols.

9. Enzyme Nomenclature and Classification

9.1. New Enzyme Subclasses: the creation of EC 1.21 and EC 2.3.3 (Dixon & Boyce)
Dixon informed the Committees of the creation of a new subdivision of EC 1, namely EC 1.21, to accommodate those enzymes where the donor comprises two different substrates that are joined by removing a H ion from each. He also circulated a diagram showing an example of such an enzyme. The other sub-subclass, EC 2.3.3, was created to accommodate transferases where the leaving group is an acyl group, which is modified during the transfer so that, when received, it is an alkyl group. Enzymes belonging to both of these sub-subclasses have recently been added to the Enzyme List.

9.2. "Enzymes" that are not strictly catalytic: EC 2.1.1.63 (Tipton)
Tipton informed the Committees that this is an enzyme that is periodically queried by members of the scientific community. When the issue was raised in 1995 by Tony Pegg, there was strong support for retaining it in the Enzyme List, especially from Bairoch, even though it does not have a catalytic turnover rate - instead, it is a DNA-repairing enzyme that methylates and then kills itself and therefore performs a single turnover before being destroyed. Barrett wants single turnover enzymes included in the Enzyme List. Degtyarenko suggested that the comment for EC 2.1.1.63 be changed to include the phrase 'this enzyme catalyses only one turnover and therefore is not strictly catalytic'. **(Action: Boyce)**

9.3. Proposed change in the comments on the stereospecificity of NAD(P)$^+$ reduction (Boyce & Tipton)
Unless one is familiar with the chirality of NAD(P)$^+$, a name or comment saying that an enzyme is 'A-specific' or 'B-specific' may hold little meaning. Boyce proposed that 'A-specific' and 'B-specific' be replaced by the phrases 'is specific for the A (*Re*)-face of NAD(P)$^+$' and 'is specific for the B (*Si*)-face of NAD(P)$^+$', respectively. Dixon approved the change of wording. Moss asked if we should go back and add this information for all enzymes involving NAD(P)$^+$. Tipton said that while this would be nice, it would not be a high priority on our list of things to do. **(Action: Boyce; Moss)**

9.4. Proposed change in the description of EC 1.x.y.z (Dixon)
The Rules for oxidoreductases (http://www.chem.qmul.ac.uk/iubmb/enzyme/rules.html), Paragraph 2, state:

> The second figure in the code number of the oxidoreductases indicates the group in the hydrogen donor which undergoes oxidation: 1 denotes a -CHOH- group, 2 an aldehyde- or keto-group, and so on, as listed in the key.

Dixon suggested changing the above wording to

> The second figure in the code number of the oxidoreductases, unless it is 11, 13, 14 or 15, indicates the group in the hydrogen (or electron) donor that undergoes oxidation: 1 denotes a -CHOH- group, 2 a -CHO or -CO–COOH group or carbon monoxide, and so on, as listed in the key.
> (this is final wording provided by Dixon after the meeting)

The reason that Dixon suggested this change is partly because there is no way that a keto group as such can be a hydrogen donor. The general principle was approved and the new wording will be implemented in the Enzyme List. **(Action: Dixon; Moss)**

9.5 Peptidases (Boyce)
Shortly before the meeting, Barrett sent a list of new draft peptidase entries, which are to undergo review before being incorporated in the Enzyme List. These draft entries will be sent to those on the JCBN mailing list and any comments on the entries should be sent to Barrett (ab9@sanger.ac.uk) and Boyce (sboyce@tcd.ie). **(Action: Boyce)**

9.6 Description of, as yet, unknown donors/acceptors (A/AH_2 & acceptor/reduced acceptor) (Tipton)
Tipton informed the Committees that EC 1.x.99.y contains two types of reaction: (1) where the receptor from model compounds takes H, in which case we use A or AH_2 to denote the oxidized and reduced acceptors. (2) For acceptors that use electrons we use the terms 'acceptor' and 'reduced acceptor'. However, as we do not specify the difference in the Rules, Tipton suggested that a Newsletter item on this topic should be prepared. **(Action: Tipton)**

Moss stated that there is a growing list of reaction schemes at http://www.chem.qmul.ac.uk/iubmb/enzyme/reaction/pending.html and pointed out the need for a mechanism to decide if they are approved and ready to be made public. Tipton suggested having them at a website where members of the Committees have one month to make suggestions - otherwise they will be made public. Dixon suggested that those considered by Dixon and Moss to be ready for publication be placed on a website for review by members of the Committees.

10. Funding Situation and Possibilities (Cammack, McNaught)

10.1 IUPAC
In order to get IUPAC approval of a document/project, one must have a project that has been pre-approved by IUPAC. The funding available for projects in nomenclature is $30,000/year. There are competitions for funding but well-framed projects tend to be approved. Cammack stated that we need to get an approved project started. Cammack has copies of project submission forms (information is required on the task chairman, task group, objectives, description of what is involved, the expected outcome, a dissemination plan, what other organizations will provide supporting funds, the precise timeframe and anticipated impact). Kazic asked about the size of such projects. McNaught said that funding would probably be at the level of $8000 for a 2-year project with 6 people involved. Wain talked about the virtual workshops that are held by HUGO. She said that they used to hold physical workshops that were attached to large meetings but said that these were not well attended. As an alternative, they advertised the virtual workshop in their bimonthly newsletter (mailing list of approximately 350 people) and on their website. They had responses within 2 weeks with 10% of the data they were looking for. The media used were e-mail and letter, and the results were displayed on their website. Cammack stated that this is an approach that the Committees should consider.

10.2 IUBMB
Cammack has corresponded with Angelo Azzi, who is our liaison in funding activities. Azzi would like to see liaison with IUPAC projects, provided that this does not impact on our meetings.

10.3. Other Possibilities
Cantor proposed that the Committees should take on the role of standardizing nomenclature to encourage interoperability between databases. For this purpose, an endowment may be possible. He recommended that the Committees approach funding bodies and the biotechnology industry to put this on a more permanent basis.

Apweiler asked what projects need to be done and what budget is needed. He said that NC-IUPHAR have a chairman for each receptor family. The NC-IUPHAR Committee just oversees the operation and does not take an active role in the work. This model involves community curation with strong editorial control. He said that he could try to find additional money for the IntEnz database and hire professional curators at the EBI to create enzyme entries. The Committees would then act in an advisory capacity. Cammack said that while the Committees need more manpower, the drafting of enzyme entries is not a simple process and is not a matter of assuming that a gene corresponds to an enzyme. Tipton stated that the drafting and curation of enzymes needs to be performed by highly skilled individuals with expertise in the many different aspects of this area so that Trinity would be a more appropriate place for such individuals to work, as training would be an integral part of the process. Apweiler said that he could raise the issue of additional funding for such curators (at the EBI only) with NHGRI, indicating that it would be easier and quicker to get funding for a supplementary project to an existing project rather than a completely new proposal.

Boyce asked Apweiler if it was his intention was to seek funding so that all Enzyme-List curation would take place at the EBI. He indicated that, as he had the master copy of the database (which was a prerequisite for funding of the Trinity group under the BioBabel project), it indeed was his intention to take over all enzyme curation and replace the efforts that are now centralized from Trinity. He indicated that the Committees could continue to have an advisory and overseeing role.

Kazic stated that a higher level of support is necessary for the group in Trinity as this is where the drafting and curation of enzyme entries should take place. She stated that, in her view, Trinity is entirely capable of maintaining a database of enzyme entries both curatorially and technically, and has been collaborating in the construction of one that will be turned over to Trinity. She reported that she has already applied for funding from the NIH that includes some support for the work on drafting enzyme entries, to be carried out in Trinity. She said that she has had indications that the project will be funded and said that the NIH would not take kindly to a request (from Apweiler) for funding for essentially the same work, even if he applied to a different body within the NIH.

11. Future Projects and Activities (items 11.1-11.3 arise from the minutes of the Köln meeting 2002)

11.1 Biochemical Compound Glossary (Moss, Kotyk etc.)
The amounts of money involved from IUPAC would not make it worthwhile writing the application. McNaught said that an interunion committee, e.g. ICSU (International Council of Scientific Unions), may be a more viable option (anticipated funding level of $100,000-150,000/project). Moss is to coordinate this project (see item 11.3 of Cologne 2002 meeting). **(Action: Moss)**

11.2 Compendium of Synonyms for Compounds (small molecules) of Biological Importance (Tipton, Kazic, Schomburg, Degtyarenko, Dixon).
Kazic and Degtyarenko were appointed as joint convenors. Several sources of information are available (e.g. BRENDA, KEGG and BND). Kazic suggested taking all sources of information and using these to get a complete dataset. McNaught said that IUPAC preferred names should be included when that project is complete. McNaught said that CAS might also be cooperative and provide information. **(Action: Kazic and Degtyarenko)**

11.3 Revision of Carbohydrate Nomenclature (Horton)

In 1996, an 80-page document on carbohydrate nomenclature was produced. The Web version (http://www.chem.qmul.ac.uk/iupac/2carb/) has had progressive modifications made to it. There was a proposal in 2002 that this document should be reviewed in 2006 (10 years after initial publication). Glycodendromers, glycoclusters, glycoproteins, neoglycoproteins, rotaxanes and catenanes should be included in the revised document. A working group, convened by Horton, is required to develop a revised document. Horton has prepared a list of carbohydrate experts that should be on the panel. Horton said that they should look at preparing a high-budget application to fund this work and that, while he is happy to cooperate at the scientific level, he does not wish to write the project proposal. He said that the work could take place during a workshop with 6-10 experts. McNaught pointed out that the project has to be funded as an IUPAC project in order for the resulting document to be classified as an IUPAC document. However, in response to a question from Tipton, who asked why IUPAC will not accept recommendations of this Committee even though they have members on our Committee, McNaught said that IUPAC do not want members of the scientific community undertaking work on their behalf that they do not want carried out. McNaught said that the carbohydrate panel could apply to IUPAC to carry out the project, but request no money from them.

11.4 Scientific Spell-checking Software (Cammack)

Cammack has had correspondence with the authors of SciProof, which is a spell-checker that plugs into Microsoft Word and checks if words are correct scientifically. The software tests if the word is correct within both the Word dictionary and SciProof. Cammack said that it does not work very well and that something more intelligent that can recognize phrases would be preferable. He provided a couple of examples of where the product is inadequate e.g., 'molecular weight' is not a term that is recommended but it does not flag it and 'pKa' is written as 'Pka'.

11.5 Bitesize Nomenclature (Cammack)

Cammack stated that we have to raise our profile in the biochemical community in order to encourage writers to use the type of nomenclature that the Committees recommend. Cammack suggested writing a series of short articles explaining terminology in simple terms, which could, in turn, have references to more detailed items (such as those in the White Book - *Biochemical Nomenclature and Related Documents*, 2nd edition, Portland Press, 1992. Liébecq, C. (Ed.) [ISBN 1-85578-005-4] and http://www.chem.qmul.ac.uk/iupac/bibliog/white.html). Cammack suggested that each person at the meeting write about one page to explain a particular area of nomenclature. According to Azzi, the Nomenclature Committee of IUBMB is entitled to one page in TiBS every month. Cammack said that this should be used for articles that can be cited. Cammack will edit these and get feedback from students before sending them to TiBS. In addition, the new series of articles could be posted on the nomenclature website. Horton said that Notes on Nomenclature was a similar venture in ACS, which lasted for a few years. The authors wrote easily digestible, concise articles. However, the journal they were published in was not widely read. Kazic suggested that an article on differences between English and American usage of terms might be useful. Dixon said that Moss has put a searchable index of past Newsletter items on the web, which would go partway to explaining such terms. Cammack will approach members of the Committees by e-mail. **(Action: Cammack)**

11.6 Any others (Cammack)

None.

12. Lipid Nomenclature

Nothing to report.

13. "Small" Molecules

This item was covered under Item 11.2. On a different issue, Kotyk raised an objection to use of the term 'pyrrolysine', which is used in EC 6.1.1.25, saying that 'pyrro' looks like a prefix to lysine. He also said that while the difference between pyro and pyrro is obvious in English, this is not the case in any other language. Dixon said that if anyone wanted to propose an amendment they should send details to Boyce.

Apweiler said that the structure of pyrrolysine is now known. Kotyk will circulate his comments to the Committees. **(Action: Kotyk)**

14. Documents and Panels

14.1 "Energases" (Tipton)

Tipton asked if a class of energases is needed or if we should redefine some of our nomenclature to cover enzymes that structurally isomerize without breaking or making a covalent bond. He said that a lot of the 'energases' could be incorporated in a new sub-subclass of isomerases. While Purich wanted to reclassify most of the transport enzymes as energases, Tipton felt that this was too radical a step. Kotyk said that Purich has a point and that we should improve our system by changing the definition of an enzyme from 'making or breaking a covalent bond' to 'making or breaking a chemical bond'. He said that ATPases and GTPases do not break covalent bonds, but that weaker chemical bonds are involved. He also said that we could reclassify the GTPases EC 3.6.1.46-EC 3.6.1.51 as enzymes in sub-subclass 3.6.4. (Acting on acid anhydrides; involved in cellular and subcellular movement), along with ATPases involved in cellular movement. He also suggested that we add a note to the header for EC 3.6.4 indicating that a covalent bond is not necessary. Purich wanted 2600 transport proteins to be included in the Enzyme List as energases, which would not sit well with our system. Tipton suggested that we have a transport ATPase subclass, with approx 15 entries in it that are not really covalent-bond-splitting enzymes. Kotyk will prepare a draft. Cammack suggested moving these enzymes out of the Enzyme List altogether and having them as an IUBMB-approved document like the transport document. Tipton was against this proposal and said that we should be incorporating such entries into the Enzyme List rather than having documents that are not part of the Enzyme List. The next stage is to list those enzymes that cannot be clearly accommodated in ATP-transport or isomerase classes. **(Action: Kotyk)**

14.2 Liaison with Journals (Elliott)

Elliott has corresponded with journal editors but little has happened as a result. Cammack said that, on looking at instructions to authors from various journals, he noticed that some make reference to the Compendium, others refer to the 1978 edition of Enzyme Nomenclature and yet others refer to Moss' website. Elliott will advise journals that some of the documents have been updated. He asked that members of the Committees let him know of specific instances of this problem. **(Action: Elliott)**

14.3 Kinases (Berman)

Kazic reported that Mike Gribskov from Susan Taylor's lab has said that he is contemplating reviewing and revising the classification of kinases but will not have time to do so before 2006.

14.4 "Molybdopterins" (Cammack)

Molybdopterins is the name given by K.V. Rajagopalan to pterins that form part of the molybdenum cofactor. Despite their name they do not actally contain molybdenum, but they bind to it. They can also bind to tungsten, hence the name is misleading. Some have one and others have two bound cofactors. While many workers in the field want the name changed to pyranopterin, Rajagopalan wants the name to remain as it is. Cammack said that he should have more news on the matter after the Gordon Conference that will be held in June 2003. **(Action: Cammack)**

14.5 Carbohydrate Nomenclature (Horton, Sharon, Merry)

Tony Merry of the Oxford Glycobiology Institute gave a presentation on a rational symbolic representation of *N*- and *O*-glycan structures. He pointed out that this is not a nomenclature scheme. He said that there is increasing interest in glycobiology among biologists but that the notation used in some standard nomenclature schemes can be daunting. Their scheme uses symbolic shapes linked into pictorial diagrams, which allows for easy recognition of carbohydrates by humans. He indicated that there are numerous schemes in use, with no two groups using the same scheme, making it difficult to compare like with like. As a result, there is a need for a universally used scheme. Unlike the Glycominds nomenclature, this is not suitable for bioinformatics as it is not computer-readable, but can be understood more readily by humans than a Glycominds representation, such as Ab3GNb3(Ab3(Fa4)GNb3Ab4(Fa3)GNb3)Ab4G. A font containing the symbols and a series of diagrams will be available for download from the Oxford Glycobiology Institute's website (http://www.bioch.ox.ac.uk/glycob/).

Horton indicated that, while Merry's notation is useful for glycoproteins, it would not translate to carbohydrates, e.g. of plants where both D- and L-forms of compounds are present and where there could be up to 100 different sugars. Cammack asked if we should recommend this scheme. Horton said that we should look at it again and then perhaps recommend it for use with glycoproteins and glycolipids. Horton and Sharon will try to have informal discussions of the system at the EuroCarb meeting in June. Horton suggested that this should be followed up at our 2004 meeting. **(Action: Horton, Sharon)**

15. Follow-up on other items from 2002 Meeting

15.1 Web Pages (Cammack)
Cammack said that he wants to rearrange Moss' website to make it more user-friendly and demonstrated the format he had in mind. Cammack said that he would do further work on his version. **(Action: Cammack)**

15.2 Minimaps (Nicholson)
Nicholson thanked the Dublin group for reviewing his minimaps. Andrew McDonald has provided links from EC numbers in the minimaps to enzymes in the Enzyme List. Nicholson said that his big map is in its 22nd edition and that the minimaps are being produced one-by-one in BAMBEd. He said that the minimaps are going to be placed on the IUBMB website. The latest edition of Powerpoint allows for animation and Nicholson demonstrated some animated minimaps (animaps), e.g., EC 2.7.1.7 hexokinase. He has also animated the glycolysis process. Nicholson has defined the term 'retrolocation' to refer to the opposite of translocation. He asked how to get this word approved. Cammack said that it was not the sort of thing that we could recommend but would depend on it being used by the public.

16. Newsletter
Cammack will distribute copies to members of the Committees. **(Action: Cammack)**

17. Publicity and Education (Elliott)
Discussed under Item 14.2.

18. Any Other Business
None

19. Date and Place of Meeting in 2004
The next meeting will be hosted by Cammack and Moss at Kings College London. The date for the meeting has not been set. The meeting concluded at 13.00 on Sunday 4 May.

APPENDIX II

Report of the Task Group on Structure Representation

Dear Alan:

As you requested in your email message of 12 Feb 2002 to Jonathan Brecher, we the undersigned have undertaken a scoping exercise to identify what kind of general guidelines for drawing chemical structures (on a computer or elsewhere) might be helpful to the community. The results of our discussion are available at
http://www.angelfire.com/sc3/iupacstructures/preferredstyles/
and the unabridged discussions themselves have been archived at
http://groups.yahoo.com/group/iupacstructures/.

Instead of simply identifying what kind of guidelines might be helpful, we have chosen to create an actual draft set of guidelines themselves (at http://www.angelfire.com/sc3/iupacstructures/preferredstyles/). We do not view this draft as anything more than a draft; we certainly do not consider it to be either complete or polished. At worst, it can be considered as our opinion of what guidelines might be helpful, annotated with examples. At best, our work might indeed become a true draft set of recommendations within an official, IUPAC-sponsored project. We are optimistic about the quality of what we have produced, but we are also extremely interested in hearing and incorporating the opinions of others.

Overall, we have tried to produce guidelines that we think are likely to be accepted by the chemistry community. For the most part, that means that our guidelines are often simply a codification of existing structure representation practices. We have tried to limit our deviations from current practice to those areas where there is a significant gain from doing so, most often because of an inherent ambiguity in some common usage. In those cases, as throughout these guidelines, we have tried to explain why a particular style is preferred rather than simply making that assertion. We have also tried to emphasize that these truly are guidelines only, and that authors should not view them as restrictive. While we hope that we have been persuasive in explaining why one style is usually better than another, we also recognize that exceptions are not only possible, but likely. Our best hope is to limit those exceptions, and never to exclude them entirely.

Our work has touched on basic issues such as the orientation of rings and the positioning of atom labels to more advanced (and sometimes controversial!) issues including the proper depiction of stereochemistry. There are some areas, including polymers and inorganic coordination chemistry, in which none of us has significant experience. Rather than propose inappropriate guidelines, we have left those areas open, and we would like to get some feedback about them from people who are more familiar with them.

In some cases, we could not decide among ourselves what would be the single best guidelines to propose. Those cases have been noted with red text, and often contain discussion of the relative merits of different options. We would be especially interested in further feedback in those areas.

As opposed to the current P-Name project, we do not expect that these guidelines will result in a single preferred structural diagram for every compound, and we have made no attempt for them to do so. We hope that these guidelines will help improve chemical communication by discouraging ambiguous and confusing depiction styles, and by encouraging clarity whenever possible.

We are satisfied with the current state of this scoping exercise. At this point, we are confident that this would be an appropriate project to be undertaken officially within the aegis of the IUPAC Division of Chemical Nomenclature and Structure Representation. Although several of us would like to remain involved in such an official project, we also request the participation of someone who is more familiar with the management and completion of such projects within IUPAC. Even in the unlikely even that our draft is accepted completely, there is still much work to be done before these guidelines can be presented to the chemical community at large. We thank you for the opportunity to work on this project to date, and hope that we can see it through to completion.

(signed)

Jonathan Brecher
Pat Giles
Harry Gottlieb
Peter Murray-Rust
Bert Ramsay
Ann Smith
Steve Stein
Keith Taylor
Bill Town
Antony Williams
Andrey Yerin

APPENDIX III

IUPAC DIVISION VIII

Division of Chemical Nomenclature and Structure Representation

Advisory Subcommittee (2004)

Dr Hidetsugu Abe (Toyohashi U of Technology, Japan)
Prof Steven M Bachrach (Trinity U San Antonio, USA; Editor, Internet Journal of Chemistry)
Dr Byron J Bossenbroek (Chemical Abstracts, USA)
Mr Jonathan Brecher (CambridgeSoft, USA)
Dr John Brennan (European Patent Office, Netherlands)
Prof Neil G Connelly (Bristol, UK)
Prof Richard Cammack (Kings, London, UK; Chairman IUPAC-IUBMB Joint Commission on Biochemical Nomenclature)
Dr Ilaria Campagnari (GSK, Italy)
Prof Chong Shik Chin (Seoul, Korea)
Prof Franco Cozzi (Milan, Italy)
Dr Ture Damhus (Novozymes, Denmark)
Prof Bernadette Donovan-Merkert (U of North Carolina, Charlotte, USA)
Prof Andreas Dress (Bielefeld, Germany)
Dr Andrey Erin (ACDLabs, Russia)
Dr Geoff Fairhurst (BASF, Germany)
Prof Henri A Favre (Montreal, Canada)
Dr Piroska Fodor-Csányi (Budapest, Hungary)
Dr Patton M Giles (Chemical Abstracts, USA; ACS Nomenclature Committee)
Dr Jonathan M Goodman (Unilever Centre for Molecular Informatics, Cambridge, UK)
Prof Richard M Hartshorn (Canterbury, New Zealand)
Dr Karl-Heinz Hellwich (Beilstein, Germany)
Prof Bernardo J Herold (Lisbon, Portugal)
Dra. Rita Hoyos de Rossi (Cordoba, Argentina)
Dr Alan T Hutton (Cape Town, South Africa)
Dr Wolf-Dietrich Ihlenfeldt (Computer Chem Center, Erlangen-Nurnberg, Germany)
Prof Aubrey D Jenkins (Sussex, UK)
Prof Jaroslav Kahovec (Prague, Czech Republic)
Prof Alan R Katritzky (Florida Center for Heterocyclic Compounds, USA)
Professor Risto S Laitinen (Oulu, Finland)
Dr Graham F McCann (Royal Society of Chemistry,UK; Editor, Dalton Trans. and J Materials Chem)
Dr W Val Metanomski (Chemical Abstracts, USA)
Prof Ebbe Nordlander (Lund, Sweden)
Prof József Nyitrai (Budapest, Hungary)
Prof Vincent L Pecoraro (Michigan, USA; Assoc Editor, Inorg Chem)

Prof C Dale Poulter (Utah, USA; Editor, J Org Chem)
Prof Damon D Ridley (Sidney, Australia)
Dr Paolo Righi (Milan, Italy)
Ms Helen Schofield (Manchester, UK)
Dr Steve Stein (NIST, USA)
Dr Keith Taylor (MDL, USA)
Dr Sarah Thomas (Royal Society of Chemistry, UK; Editor, ChemComm)
Mr Kevin Thurlow (LGC Nomenclature Advisory Service, UK)
Dr Edward S Wilks (ex-Dupont, USA)
Dr Janusz L Wisniewski (MDL, Germany)
Dr Shen-Gang Yuan (Shanghai, China)

Appendix IV

Nomenclature World Wide Web Database – Statistics

Statistics based on log of IP addresses used each day. Total usage to date about 2411000. Data on 179 countries recorded so far. Summary data for 1996-2003 at www.chem.qmul.ac.uk/iupac/usage/ For full details of each document see www.chem.qmul.ac.uk/iupac/ or www.chem.qmul.ac.uk/iubmb/

Average use **per week**

Year	1996	1997	1998	1999	2000	2001	2002	2003	max
Total usage	296	650	1476	2786	5515	9813	15360	19081	22208
Search Facility	-	-	-	204	1663	4169	8355	11447	13872
Bibliographic Data	-	61	142	235	325	470	598	652	790
Map of Usage	-	7	8	29	37	58	83	74	138
IUPAC Nomenclature									
Class Names Glossary	138	157	430	693	1039	1504	2178	2483	3137
Physical Org Chem Glossary	29	36	136	343	751	1089	1796	1986	2487
Atomic Weight	23	48	95	144	310	651	964	1264	1712
Periodic Table	-	-	-	17	155	291	475	740	1033
Stereochemical Glossary	-	32	85	135	231	392	602	659	884
Bioinorganic Glossary	-	-	61	108	201	391	633	600	799
Medicinal Chemistry Glossary	-	-	56	87	150	316	532	581	668
Section F (Natural Products)	-	-	-	14	121	321	450	484	633
Fused Ring	-	-	64	73	110	198	241	268	370
Ions and Radicals	-	-	-	-	72	150	196	220	373
Numerical Term	-	18	27	35	54	99	150	174	224
Gold Book	-	-	-	-	80	127	155	166	222
Hantzsch Widman	12	14	31	46	56	89	116	116	147
von Baeyer	-	-	-	29	61	106	130	115	211
Phanes	-	-	31	42	56	80	95	114	187
Fullerenes	-	-	-	-	-	-	69	114	161
Spiro	-		-	26	47	90	114	111	220
Delta Convention	8	9	19	30	54	82	110	106	163
Section H (Isotopic Label)	-	-	26	34	46	73	90	84	144
Element Name > 100	-	-	-	20	45	78	87	83	163
Lambda Convention	6	8	17	28	40	60	76	71	111
Phane II	-	-	-	-	-	-	-	58	75
Guide Errata	-	-	-	20	21	25	32	47	61

IUPAC/IUBMB Nomenclature

Steroids	12	21	87	93	396	811	1213	1660	2370
Carbohydrates	46	72	144	237	453	835	1156	1477	1848
Amino Acids & Peptides	31	62	135	186	359	670	1072	1357	1721
Vitamin B-6	-	-	-	34	95	155	267	514	721
Vitamin B-12	-	-	-	49	69	146	266	359	640
Folic acid	-	-	-	60	58	210	208	330	484
Tocopherol	-	-	21	33	48	80	150	283	404
Nucleic Acid Abbreviations	-	-	-	45	77	136	202	242	403
Lipids	-	-	-	29	70	132	198	224	297
Tetrapyrroles	-	-	-	-	-	124	221	223	349
Vitamin D	-	-	-	-	47	69	125	204	295
Glycoproteins	-	-	20	32	71	134	172	192	311
Polypeptide Conformation	-	8	14	34	61	111	173	185	394
Cyclitols	-	-	21	51	72	113	174	182	309
Glycolipids	-	-	15	35	65	91	137	151	292
Biochemical Phosphorus	-	-	-	-	62	103	151	149	276
Carotenoids	-	-	-	-	46	84	128	141	187
Polysaccharide Conformation	-	8	14	26	49	82	134	136	292
Lignans and Neolignans	-	-	-	-	-	71	123	128	205
Retinoids	-	-	-	-	35	71	99	127	177
Quinones with Isoprenoid Chain	-	-	-	-	-	47	90	103	138
Polynucleotide Conformation	-	7	15	27	44	68	92	94	122
Polymerised Peptides	-	-	-	-	34	56	91	93	142
Prenols	-	-	-	19	33	55	77	83	121

	1996	1997	1998	1999	2000	2001	2002	2003	max

Both Committees

Committees' Homepage	18	38	65	123	268	423	653	763	946
Newsletter	-	-	25	59	145	304	456	436	635

IUBMB Nomenclature

Enzymes	16	54	124	320	1086	2088	3560	4099	4985
EC 1	-	-	-	35	241	487	922	1034	1294
EC 2	-	-	-	-	180	438	769	872	1105
EC 3	-	-	-	-	165	427	947	1011	1352
EC 3.4 (50 file)	16	54	>82	200	285	281	184	123	-
EC 3.4 (single)	-	-	-	-	-	134	343	375	591
EC 3.4 (total)	-	-	-	-	-	336	484	461	706

EC 4	-	-	-	-	90	223	410	403	569
EC 5	-	-	-	-	64	164	294	288	441
EC 6	-	-	-	-	46	138	239	238	342
reaction	-	-	-	-	48	119	381	585	726
newenz	-	-	-	-	53	60	75	66	151
Enzyme Supplement 5	-	-	42	66	79	53	37	30	-
Enzyme Kinetics	-	-	16	61	152	249	365	435	784
Electron Transport Proteins	-	-	-	-	58	107	163	166	224
Membrane Transport Proteins	-	-	-	-	-	-	93	153	197
Biochemical Thermodynamics	-	-	22	40	66	107	132	142	200
myo-inositol	-	-	11	23	43	74	125	134	225
Incomplete Nuc. Acid Sequence	-	9	20	31	50	75	103	129	162
Isoenzymes	-	-	14	28	68	106	124	126	216
Branched Chain Nucleic Acids	-	3	6	10	40	63	115	118	185
Peptide Hormones	-	-	-	-	32	51	80	99	116
Multienzymes	-	-	10	13	18	25	37	36	53
Translation Factors	-	-	-	-	11	18	34	34	49

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