

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

Cambridge, UK January 26, 2002

Members Present: Dr Michael Dennis, Dr Stephen Heller, Prof Michael Hess, Prof Herbert Kaesz, Dr Alexander Lawson, Prof G. Jeffery Leigh, Dr Alan McNaught (President), Prof Bruce Novak, Dr Warren Powell (Secretary), Dr William Town, Dr Antony Williams

Members Absent: None.

The first meeting of the Division Committee of the new IUPAC Division of Chemical Nomenclature and Structure Representation held at the offices of the Royal Society of Chemistry, Thomas Graham House, Science Park, Milton Road, Cambridge, UK was convened by President Alan McNaught at 9:00 a.m. on Saturday, January 26, 2002.

1.0. President McNaught welcomed the members to Cambridge and specifically to the offices of the Royal Society of Chemistry. Each of the members introduced himself and provided a brief bit of background information. Housekeeping details for breaks and lunch were announced and an invitation for dinner at the President's home was given.

2.0. The agenda as circulated was approved without additions or modification.

3.0. Division Business

3.1 The Terms of Reference for Division VIII as agreed by Council (Appendix I) were discussed.

- (1) The Terms of Reference should be kept general. Specific instructions should be avoided. At the beginning of item 6, the phrase "As far as possible..." should be added.
- (2) In answer to a question about the interaction of Division VIII with ICTNS (formerly IDCNS) it was explained that interaction regarding nomenclature recommendations and reports would be in the same manner as in the past for any other Division. After approval of recommendations and reports by our division, they will be forwarded to ICTNS and will pass through the established review processes.
- (3) In addition to the Advisory Subcommittee, the Division VIII Committee is entitled to six National Representatives to assist in carrying out the Division's responsibilities as given in the Terms of Reference. At the moment we have more nominations than six for National Representative positions. It was agreed that, after those accepted as Division Committee National Representatives have been notified by the Secretariat, the rest should be invited as members of the Advisory Subcommittee.

3.2. Division Rules (Appendices II and III). As a new division, we must consider whether or not we will have Division Rules. Divisions may adopt Rules but are not required to do so. Recognizing that existing Division Rules need revision, the

Secretary General has prepared guidelines (Appendix II) and a model for a set of Division Rules (Appendix III). The following comments were offered regarding the model set of rules.

- (1) Item 1 would be modified in accord with item 1 of the Terms of Reference. The name of the Division is the Chemical Nomenclature and Structure Representation, a slight change from the name announced earlier; the word Chemical has replaced the word Systematic.
- (2) It was felt unrealistic for the nominating committee to have only two experienced and three inexperienced members. Therefore, the following motion was made, seconded, and passed unanimously. "Under Rule 5(a) the composition of the five-member nominating committee should consist of *three* members of the existing Division Committee and the other *two* chosen from outside of IUPAC on the basis of the breadth of their expertise." This would need Bureau approval.
- (3) Under 5(c) delete "from academia, government and industry".
- (4) A change of "under procedures defined by the IUPAC Secretariat" to "under fair practices defined by the IUPAC Secretariat" was proposed.

Members were asked to send further comments on the model Division rules as modified as above. After an appropriate amount of time for comments, the proposed rules for our Division will be submitted to the members by e-mail for approval and then to the Bureau in September.

- 3.3. Division Electorate. Discussion of the "Extract from the minutes of the 41st Council Meeting, Brisbane, July, 2001" (Appendix IV) concluded that, in addition to the Titular Members, Associate Members, and National Representatives, the members of the Advisory Subcommittee and current Task Group Chairmen should be members of the Division Electorate. This should be proposed to the Bureau for inclusion in our Division Rules (see item 3.2).

4.0. Advisory Subcommittee.

- (1) Terms of Reference are given in Appendix V.
- (2) As of December 6, 2001, the Advisory Subcommittee consisted of 36 members given in Appendix VI. The following were suggested as additional members: Prof. Piroška Fodor-Csányi (Hungary), a long-time member of CNIC; Prof. Bernadette Donovan-Merkert (USA), current Chairperson of the ACS Inorganic Chemistry Division's Nomenclature Committee; National Representatives nominated for membership on the Division Committee, but not appointed (see also item 11.5). M. Dennis would approach K. Schwall, currently head of the CAS Authority Database Operations Department to ascertain his interest.

5.0. Matters Arising from the Minutes of the July, 2001 meeting of the Committee on Chemical Identity and Nomenclature Systems (available as a separate item on the Division WebBoard)

- (1) Item 3.0. The reason for the name change from the Division of Systematic Nomenclature and Structure Representation to the Division of Chemical

Nomenclature and Structure representation was to ensure that all nomenclature matters dealing with chemical compounds would be included, not just systematic nomenclature.

- (2) Item 5.1.1. The Laboratory of the Government Chemist was asked if they wished to be added to the IUPAC Web page as a source for nomenclature assistance. Interest was expressed but no suggested text was sent. The question of adding other sources of nomenclature assistance, such as the Chemical Nomenclature Service (Gustav Penzlin), and other consultants, with an appropriate disclaimer, to the Web site was discussed. It was finally decided to recommend that the Web site provide links only to free services, such as ACD, MDL, and CAS, where appropriate, with a suitable disclaimer.
- (3) Item 5.1.2.2. Several authors of translations of IUPAC recommendations had been included as Advisory Subcommittee members, and the Division Committee would continue to try to establish contact with such people.

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

- (1) JCBN will remain as a Commission of Division VIII for two years. There is some pressure for it to evolve into a project based operation under Division VIII. A project driven system is difficult to work out when two unions that differ in operational aspects are involved. The Chairman would like to have an operational proposal for JCBN by its meeting in May, 2002. He will meet with the current JCBN/ NC-IUB Chairman with the aim of developing a proposal for discussion by Division VIII and to present to the Bureau in September.
- (2) JCBN meets annually with the Nomenclature Committee of the International Union of Biochemistry and Molecular Biology (NC-IUB). G. Moss summarized the current projects of JCBN. The main project of JCBN continues to be the Enzyme List, which is now all on the Web. Every two months new enzymes are put up on the web for discussion. A new complete list appears on the Web about every eighteen months.

“Nomenclature for Lignans and Neolignans, Recommendations 2000” has appeared in PAC, **2000**, 72, 1493-1532. “Nomenclature of Cyclic Peptides, Recommendations, 1998” is to be submitted for ICTNS and public review.
- (3) Future projects include finalization of a draft of nomenclature for prostaglandins and thromboxanes and development of a specific proposal for documenting nomenclature for miscellaneous compounds of biochemical interest.

7.0. Current Division VIII Projects.

- 7.1. The IUPAC Chemical Identifier (ICHI). The IUPAC Committee on Chemical Identity and Nomenclature Systems (CCINS) identified the need for an open, extensible, standard means of representing chemical substances. In response to this need a project has been initiated to develop an IUPAC Chemical Identifier. A general description of this project can be found at the IUPAC website (<http://www.iupac.org/projects/2000/2000-025-1-800.html>). The ICHI is intended to plug into commercial naming programs. At the present time the development work is funded by NIST. An α -file is now in hand and it is hoped that a β -version will be ready

for distribution by the end of March. In response to questions about tautomers and stereochemical considerations, S. Heller provided the responses given in Appendix VII.

7.2 Preferred Names in the Nomenclature of Organic Chemistry. The next revision of *Nomenclature of Organic Chemistry* (the IUPAC "Blue Book") will provide recommendations for selecting a "preferred name" in addition to continuing the development of organic chemical nomenclature. Previously, although IUPAC recommendations have limited the choice of names available for particular substances, in many cases alternatives have been allowed and IUPAC has not always expressed preferences. However, for many areas of work, particularly where there is a regulatory or other legal requirement, there is a need for a single internationally approved chemical name. It is this need that the current revision of the Blue Book is intended to fulfill, by defining selection rules to arrive at a preferred name for any organic chemical structure. Thus, the new recommendations will continue to describe a variety of recognized nomenclature systems, but will also contain selection rules enabling preference to be expressed, for example, between "decahydronaphthalene" and "bicyclo[4.4.0]decane", or between "1-ethoxypropane" and "ethyl propyl ether". The idea is that anyone needing to choose among alternative IUPAC names for any purpose (not only regulatory) would be at liberty to use these selection rules.

The revised Blue Book is expected to have eleven chapters. At the present time a complete draft of all chapters has been completed running to nearly 1000 manuscript pages. A second draft of the first two chapters has been completed and the third chapter is in the process of revision. A project extension has been approved; the project number is 2001-043-1-800. Since the revised edition of *Nomenclature of Inorganic Chemistry* (the IUPAC "Red Book") is not expected to provide preferred names for noncarbon compounds, a project called Alignment of organic and inorganic preferred names (see 7.4) is attempting to assist in parts of the revised organic book where noncarbon compounds are given names on which organic derivatives are based. (a meeting of this Task Group will be held tomorrow in Cambridge).

There was objection to the term "preferred" names. "Regulatory" and "standard" were suggested as alternates. A search for a better term will include a note to be placed on the Division webboard requesting alternatives.

It was felt that the best possible scenario would be to have preferred names in both the organic and the inorganic books and that the books come out together. However, this would significantly delay both books; the revised Red Book is under contract with the Royal Society of Chemistry (see 7.3) and it is hoped that the revised Blue Book will be published by the end of 2003.

For review purposes, it was proposed that the next draft of the organic book be put on the webboard. Final publication in electronic form vs. a printed version should be discussed by the Publications Committee.

Although preferred names for noncarbon compounds is expected to be a project when the revised Red Book is finished, the question of how to proceed regarding preferred names for polymers requires further discussion.

The establishment of commercial nomenclature programs for inorganic or polymers is quite unlikely simply because there is no market for names in these areas. Many biochemical names are included with organic programs.

7.3. Inorganic Chemical Nomenclature. There is a contract with the Royal Society of Chemistry for publication of a revision of *Nomenclature of Inorganic Chemistry* (the IUPAC "Red Book"). The revision must go forward; the 1990 edition of the Red Book is out-of-print. It is hoped that the revision can be accomplished by the end of the year. Consultation with organic nomenclaturists with regard to names of organic ligands and principles of substitutive nomenclature must occur, some of which is happening this weekend here in Cambridge. Preferred names will not be included in the revision.

7.4. Alignment of organic and inorganic preferred names (Project 2001-031-1-800). Following an initial meeting of the task group at the end of September, 2001, a proposal outlining a possible division between the responsibility for naming compounds containing the elements Al, In, Tl, Ge, Sn, Pb, Sb, Bi, and Te was circulated to the members of the alignment group. It is one of the main items for discussion at the meeting of the group to be held tomorrow (January 27) here in Cambridge. If agreement on its basic principles can be achieved, even if it is not possible for preferred names to be in the revised Red Book, it will provide the necessary guidelines for appropriate parts of the revised Blue Book to be completed.

Other topics include the use of the word hydrogen in names of partially deprotonated acids and esters.

In addition, assistance in naming organic ligands for naming inorganic coordination compounds will be provided.

7.5. Fullerene nomenclature, Part II (Project 2001-014-1-800). A meeting of the Task Group for preparing a second part of the nomenclature of fullerenes was held on January 23-24 in Zürich, Switzerland. Its first order of business was to finalize the comments from the IDCNS and public review of the first fullerene paper "Nomenclature for the $C_{60}-I_h$ and $C_{70}-D_{5h(6)}$ Fullerenes (IUPAC Recommendations 2002)". This paper should be ready for publication by the end of February.

A initial draft for a second paper on fullerene nomenclature by F. Cozzi was reviewed and agreement was reached on four classes of fullerenes to be studied, the first two classes encompassing two types of fullerenes with axial symmetry, one with a contiguous spiral pathway for numbering and one without; fullerenes with C_s symmetry; and fullerenes with C_i or C_1 symmetry. F. Cozzi will redraft his initial draft to cover the first two classes (types). Additional examples of fullerenes with axial symmetry but without contiguous spiral pathway for numbering, besides the [3,8]- and [3,10]fullerenes given in CAS documentation, are needed. An alternative for numbering the $(C_{54}-C_s)[5,6]$ fullerene given in the CAS documentation was found. It will be investigated with other C_s -fullerenes. Finally, it was found that the $(C_{34}-C_1)[5,6]$ fullerene and the $(C_{48}-C_1)[5,6]$ fullerene used in CAS documentation had a C_2 axis and were therefore not C_1 ; a true C_1 will have to be studied.

Numberings for the known [5,6]fullerenes, $C_{76}-D_2$, $C_{78}-D_3$, $C_{78}-C_{2v}$, $C_{80}-D_2$, $C_{84}-D_2$, and $C_{84}-D_{2d}$, will be investigated to determine what new rules might be needed for these fullerenes with axial symmetry.

7.6. Structure Based Nomenclature for Cyclic Macromolecules. A supplementary Project Submission Form is in the process of preparation. The latest draft of the document itself has not yet been received. There was some concern about the term

macromolecules in the title in that it could be interpreted to mean just large rings rather than rings containing polymeric units.

- 7.7. Nomenclature for Rotaxanes and Catenanes. This project has been separated into two projects, one dealing with macromolecular rotaxanes and catenanes and one with molecular rotaxanes and catenanes, i.e., discrete molecules. A supplementary Project Submission Form is needed for the former and a new Project Submission Form for the latter. T. Wilks was suggested to also be the task group leader for the molecular rotaxane project; other participants suggested were G. Moss, V. Metanomski, and A. Erin.

It was also suggested that it would be best if the two documents were published together, even though the macromolecular document appears to be further along.

- 7.8. Nomenclature of Dendrimers and Hyperbranched Oligomers and Polymers. A supplementary Project Submission Form is in the process of preparation. The latest draft for this project is dated August 2001.
- 7.9. Process-Based Nomenclature for Modified Polymers. The name for this project has been changed to Nomenclature for Chemically Modified Polymers; a supplementary Project Submission Form is being prepared. The latest draft is dated October 2001.
- 7.10 All of the above macro documents (7.6-7.9) are due to be discussed in Beijing, July 2- 5, 2002. B. Novak will represent Division VIII at these discussions.
- 7.11. A feasibility study for a revision of the list of macromolecular abbreviations is planned. This would become a new task and remain with Division IV.

8.0. Future Division VIII projects.

- 8.1. Organometallic Nomenclature. A Project Submission Form is being prepared by H. Kaesz and W. Powell. A general chapter by A. Salzer has already been published (PAC **1999**, 71, 1557). Other topics to be included are metallacycles, rings or ring systems that contain at least one metal atom, and "ocenes", such as ferrocene. It is hoped that this project will result in a book on organometallic compounds, the color of which has not been decided, perhaps blue and red stripes.
- 8.2. Preferred Names for Inorganic Compounds. In Washington, D. C., CCINS suggested that CNIC seriously consider a preferred name project for the Red Book. Since preferred names will not be included in the current revision of the Red Book, Project Submission Form is needed. T. Damhus was suggested as a person to set up such a task group. Presumably this would lead to a new edition of the Red Book in a few years.
- 8.3. Stereochemistry. Currently there are two projects involving stereochemistry, one of which is Chapter 8 for the revised Blue Book (H. Favre) and the other is a revision of Section E of the *Nomenclature of Organic Chemistry*, a project begun under CNOC under the convenorship of B. Bossenbroek. To complete the latter project, a supplemental Project Submission Form is needed. It was suggested that G. Moss prepare such a supplemental form with the assistance of B. Bossenbroek.

A question was asked as to how to deal with inorganic stereochemistry. The revision of section E would cover inorganic stereochemistry only insofar as needed for

elements such as sulfur, phosphorus, and perhaps arsenic. R. Hartshorn was suggested as a member of the task group for revision of Section E.

Clearly, other areas of stereochemistry need to be developed. It was decided to undertake a scoping exercise to gather information about stereochemical needs across all areas of chemistry, organic, inorganic, macromolecular, organometallic, biochemical. R. Hartshorn was suggested as a leader of an exercise with G. Moss and B. Bossenbroek assisting to explore what IUPAC and other organizations have on stereochemical nomenclature and what is needed.

A need for standard drawing conventions for stereochemical structures was discussed. Examples were given showing ambiguous or confusing stereochemistry drawings. A basic question was raised regarding representation of stereochemistry in computer files, namely, at what point do the atomic coordinates for stereochemical descriptions become important? It was eventually decided to ask Jonathan Brecher, of the Cambridge Software Group to lead a group charged with collecting together existing guidelines from standards bodies and other organizations, look for commonality of approach, and identify areas where guidance from IUPAC could be useful. Initially, this study could be restricted to the ways in which structures can be represented graphically on a computer screen. Tony Williams, Sandy Lawson and Michael Dennis (members of the Division VIII Committee) would be appropriate points of contact with ACD, MDL and Chemical Abstracts, respectively. Other possible sources of information would be the IChI task group and WHO.

From the above two scoping exercises it should be possible eventually to define a project or projects to be funded by Division VIII.

- 8.4. Java Applet for Stereochemical Assignment. The algorithm for the assignment of stereodescriptors for organic compounds has been completed and published by J. Wisniewski in *Macromolecules*, **2001**, *6*, 915-926. A. McNaught would ask the author whether he was now in a position to develop a Java applet for IUPAC.
- 8.5. Phane Nomenclature, further development. Phane II: Substitution Derivatives of Phane Parent Hydrides is nearing completion; it should be sent to the IUPAC Secretariat for publication by the end of March. So far, this powerful new type of nomenclature has been applied to large systems where the 'super atoms' are rings or ring systems. However, many other structural fragments could be imagined as 'super atoms'. Possible applications need to be found for evaluation. W. Powell will write to Prof. Takemura, a co-editor of a book called *Cyclophanes in the 21st Century*, for which H. Favre and W. Powell wrote a short chapter outlining phane nomenclature, to try to find out the type of structures that will be included in this book.
- 8.6. Boron Nomenclature. Neither the revised Red Book nor the revised Blue Book will contain a comprehensive documentation of nomenclature for boron compounds, which range from organic heterocycles to boron hydrides, neutral and ionic, and addition compounds, cyclic and acyclic. Two books, *Inorganic Chemical Nomenclature*, by B. P. Block, W. C. Fernelius, and W. Powell and *Nomenclature of Organic Compounds*, 2nd edition, by R. B. Fox and W. H. Powell contain extensive documentation on nomenclature of boron compounds, and there is a series of papers by J. B. Casey, W. J. Evans, and W. H. Powell containing systematic proposals for naming boron hydrides. A project is needed to form a task group to document comprehensively nomenclature

for boron compounds, which require both organic and inorganic nomenclature principles. There is a real need for researchers in the field to become involved with boron nomenclature.

- 8.7. Solid-state Nomenclature. The need for a project for revision and/or extension of Red Book chapter 6 was raised. A. McNaught will contact R. Metselaar concerning such a need.
- 8.8. Computer-aided Cluster Nomenclature. A. Dress has been working on such a project within CNIC. The present status of his work is unknown. A McNaught would contact him to ascertain his present interest. In his work a name is mathematically based.
- 8.9. Synonym Database for Compounds in Common Biochemical Usage. The Chairman of JCBN is interested in such a project. A. McNaught will discuss with him how to proceed. Constraints need to be defined. There are questions that need answers, e.g., should such a database include acronyms, SDF files?
- 9.0. General and structure-type formulas for minerals, etc. H. Kaesz received a request from Prof. Peter Bayliss that IUPAC should recognize the scheme for representation of structural formulas used in the Mineral Powder Diffraction File. A. McNaught wrote to Prof. Sidney Abrahams about this request. The correspondence is given as Appendix VIII. It was decided to respond to say that we will not do anything until the IUCr Commission on Crystallographic Nomenclature has been consulted.
- 10.0. CAS/IUPAC Conference on Chemical Identifiers and XML for Chemistry. M. Dennis distributed a preliminary announcement (see Appendix IX) concerning the conference as given in the above heading to be held July 1, 2002 at the Pfahl Executive Education and Conference Center and The Blackwell in Columbus, OH.
- The day before, June 30, a meeting of the IChI group for a review of the project will be held in Columbus.
- S. Heller summarized the XML (eXtensible Markup Language) meeting held during the previous two days here in Cambridge. Further information may be found in a column by Tony Davies in *Spectroscopy Europe*, **2002**, 14(1), 22-24 (attached as XML-Article-Cambridge.pdf). A project to develop standard XML data dictionaries is being put together, based on existing IUPAC glossaries. S. Stein is the project leader.

11.0. Divisional Modus Operandi

- 11.1. Division Committee meetings. Since it seemed advisable to have a second meeting this year given that we are just getting a whole new Division organized, it was suggested that we meet in Boston, MA, USA around the time of the ACS meeting, August 18-23. The ACS Committee on Nomenclature will hold its annual meeting on August 17 and an open meeting on August 19, and it might be nice for our Committee to have some interaction with the ACS Committee. W. Powell and M. Dennis will look into arrangements for the Division Committee to meet in Boston during the period August 15-20.

There will be Divisional Committee meetings during the General Assembly in Ottawa, August 10-17, 2003. Council meets August 16-17, 2003.

- 11.2. Project Group Meetings. Project group leaders should be urged to try to have a meeting near or at the time of the General Assembly in Ottawa.
- 11.3. Document review and the Role of ICTNS (formerly IDCNS). A general discussion about review of documents and the role of Divisions and of IDCNS (now ICTNS) is attached as Appendix X. The Chairman will continue to be T. Cvitaš and the new Secretary is Bernado Herold. Besides a Titular Member representing each Division, additional Titular Members will assist the Chairman and Secretary in reviewing Recommendations and Technical Reports. V. Metanomski and J. Lorimer will assume this responsibility. T. Damhus will also assist in this review.
- It was suggested to propose to ICTNS that an integral part of the Division VIII review procedure would involve making documents available to all members of the Advisory Subcommittee for download from the Division VIII webboard.
- 11.4. Communications. The IUPAC8-1 listserver provides a means of communication among the Division Committee. It is not strictly confidential so we must take care about what we share.
- The Division Webboard (<http://webboard.rsc.org:8088/~IUPACVIII>) is available to both Division Committee and Advisory Subcommittee members for communication and posting current draft recommendations. Attachments should be posted as .rtf or .pdf files.
- In view of problems experienced by some Committee members in reading files attached to e-mails, A. McNaught would set up a repository for file autdownload.
- 11.5. Involvement of the Advisory Subcommittee. The Advisory Subcommittee should be able to be kept informed by means of the Webboard.
- Additional members for the Advisory Subcommittee were suggested, to be contacted by A. McNaught.
- 11.6. Development of Project Proposals and general publicity. It is necessary to make known that anyone can bring up or start a project by submitting a proposal. The forthcoming article by A. McNaught in Chemistry International is a start. The possibility of publishing other articles in national magazines, such as Nature and Chemistry and Engineering News, should be pursued. W. Town would make arrangements for an article about the new Division in the Alchemist (ChemWeb). The macromolecules list server could be useful for publicity; B. Novak will send details to M. Hess. Lectures, talks, and powerpoint presentations would be useful. S. Lawson will act as a collection point for publicity-type presentations on nomenclature; members should send him anything they have available.
- 11.7. Composition of Project Groups. Concern was expressed about excessive size of project groups; however, it was expected that budget restraints would impose a degree of self-regulation.
- 11.8. Involvement of National Adhering Organizations. It is very desirable to have as much input from National Adhering Organizations as possible. We should ask John Jost to ask all National Adhering Organizations to put us in contact with appropriate nomenclature and education committees in their countries. A. McNaught would make a similar request to Advisory Subcommittee members.

12.0. Other Business. G. Moss distributed statistics regarding the usage of his world-wide web nomenclature database. As of mid-January, they given in Appendix XI.

Submitted: March 8, 2002

Warren H. Powell
Secretary

Approved: March 11, 2002

Alan D. McNaught
Chairman

APPENDIX I

IUPAC Division of Chemical Nomenclature and Structure Representation

Terms of Reference

The Division is responsible for maintaining and developing standard systems for designating chemical structures, including both conventional nomenclature and computer-based systems. This responsibility is to be fulfilled by:

1. Identifying the needs of the user community.
2. Generating projects arising from those needs.
3. Identifying project leaders and task groups to carry out the work.
4. Administering approved projects financially, monitoring their progress, and approving resulting recommendations for review by established IUPAC procedures.
5. Identifying new sources of expertise and enabling their involvement in projects.
6. Ensuring that nomenclature systems projects and the resulting recommendations are compatible with each other, with established IUPAC recommendations, and with computer-based systems for manipulating chemical names and structures.

APPENDIX II

EC Agenda Item 6

New Division Rules

The Division Rules are badly out of date. I have prepared a model set of Rules, which each Division can adapt as needed. At present we await action by the Division Committees as a result of the following message. No action is required by the EC.

January 5, 2001

To: Division Presidents

At Cobham we discussed updating the Rules of the Divisions, and I presented a model set of Rules. I have received a suggestion for a few changes in the Model Rules, which I have incorporated and send to you as an Attachment. Let me remind you of several points discussed in Cobham:

1. Statute 10.3 permits Divisions to adopt Rules, but it does not require Rules. If such Rules are adopted, they must be approved by Council; hence changes in Rules must also be approved by Council. Over the long term, this process provides some stability and prevents a particular Division Committee from making changes abruptly. By the same token, the process prevents a Division Committee from responding quickly.

2. If a Division wishes to formulate Rules and to have them approved by Council in Brisbane, we need to include the proposed Rules in the Council agenda book, which will be sent out by May 1. If there are minor changes in wording adopted in Division Committee meetings in Brisbane, we could probably persuade Council to approve the revised version. However, we should avoid having to print any extensively revised Rules hastily in Brisbane and distribute them to the Bureau and Council at the last minute. A number of "late papers" used to be provided frequently, but we have managed to avoid that in the last few years, and I do not think it reasonable to inundate Bureau members or Council delegates with a lot of paper for consideration without time to study the issues.

3. If you do prepare Rules, you are free to write what you wish, but I hope that the Model can be followed as much as possible. Don't forget that your Division's Terms of Reference are a part of the Rules, so these should be updated as needed.

4. It may be that some Divisions are not quite ready to agree on new Rules in time for action in Brisbane. If so, you might - as an interim step - want to adopt the wording of the Rules as Division "policy". This could be changed as needed or might be used to propose formal Rules in 2003.

Please keep John Jost or me informed as to your progress and decisions. Let me know if I can be of any help.

Best wishes,

Ted

APPENDIX III

MODEL B January 5, 2001

_____ **Division**

DIVISION RULES

1. The mission of the _____ Division is to promote pure and applied _____ chemistry. Terms of Reference are attached.
2. Under the Statutes, Bylaws, and policies of the Union, the Division is managed by its Division Committee. S10 and B4.1 and their subsections are particularly relevant. The Division Committee is responsible for initiating and managing scientific projects, symposia and other activities within its area of responsibility and for cooperating with other Divisions in initiating and managing interdisciplinary projects, symposia and other activities.
3. The composition of the Division Committee and terms of service of its members are given in B4.103. In addition, under policy established by the Bureau, up to six National Representatives may be elected to the Division Committee.
4. (a) Titular Members of the Division Committee are nominated and elected by the electorate defined in B4.103. Candidates for titular membership are nominated by the Nominating Committee described below.

(b) Associate Members may be elected by the Division Committee, as provided in B4.103.

(c) National Representatives are elected by the Division Committee on nomination by National Adhering Organizations, according to procedures defined by the Bureau.

(d) Interim appointments to fill vacancies on the Division Committee occurring between meetings may be made by the Division President for terms ending at the end of the year in which the next General Assembly is held.
5. Candidates for Titular Member of the Division Committee are named by a Nominating Committee, prescribed by IUPAC policy and procedures defined by the Bureau, as follows:
 - (a) The nominating committee consists of five members [subject to an exception by the Bureau], with no more than two members from the existing Division Committee and the other three chosen from outside IUPAC on the basis of the breadth of their expertise. The Division President will not be a member of the Nominating Committee.
 - (b) The Nominating Committee is appointed by the Division President with the concurrence of the IUPAC Executive Committee.

- (c) Nominees should be scientists from academia, government and industry with the expertise and experience necessary to maintain a Division Committee with appropriate scientific stature and breadth. Categories of vacancies may be established by the Division Committee if desired to ensure diversity in subject matter, geographic distribution, or other characteristics. More than one nominee for each vacancy is desirable but not required.
6. Elections shall be conducted by e-mail (or ordinary mail as necessary) under procedures defined by the IUPAC Secretariat.
 7. The Officers of the Division, as prescribed by B4.103 and B4.104, are President, Vice President (designated as President elect), and Secretary, with the immediate Past President serving as a Titular Member. With the advice of the President of the Union, Officers of the Division are elected by the Division Committee, subject to final approval by the Council. The Officers together form an Executive Committee to act for the Division Committee between meetings. The duties of the Officers are as follows:
 - (a) The President is the administrative head of the Division, presides at meetings of the Division Committee, and is an *ex officio* a member of all bodies of the Division. The President serves as a member of the Bureau and is the principal representative of the Division within and outside the Union.
 - (b) The Vice President acts for the President in his absence, assists the President as requested, and serves on the Division executive committee. He shall assume the office of Division President in the event of the President being unable to perform the functions of that office, without prejudice to the forthcoming period of office as President.
 - (c) The Secretary assists the President in carrying out the business of the Division and maintains the records of the Division.
 8. (a) The Division Committee may establish and the Division President may appoint subsidiary bodies, such as working parties and advisory groups, which will have the status of Division subcommittees, as described in S 10.6. Task groups may be formed to carry out specific projects. The terms of reference or charge to each group, as well as its lifetime, shall be established by the Division Committee.
 - (b) The Division Committee may propose to the Bureau the establishment of Commissions, with terms of reference and lifetimes, under the provisions of B4.301.
 - (c) The Division Committee and Division President will exercise responsibility and oversight over all bodies created under parts (a) and (b).
 9. These Rules may be amended by the Division Committee, subject to approval by the Council.

APPENDIX IV

Extract from minutes of the 41st Council meeting, Brisbane, July 2001

12. Proposed Changes to Statutes and Bylaws

12.1. Revision of Bylaw 4.103 - Division Electorate – Bureau

Dr. Becker noted that with the dissolution of Commissions at the end of 2001, the electorate for the Division Committees as defined in the Bylaws would, in most cases, be reduced to the current members of the Division Committee. After much discussion at the Division Presidents meeting in 2000 and the subsequent Bureau meeting, the Secretary General was asked to draft an amendment to the Bylaws to accomplish what the Division Presidents and the Bureau had agreed. The current amendment defines part of the electorate, and gives the Bureau the power to define the rest of the electorate. This was done to allow flexibility as IUPAC gains experience with the new system. The text of the changes proposed is as follows:

B4.103 The Titular Members of each Division Committee shall be chosen by an electorate comprising the Titular Members, Associate Members and National Representatives on the Division Committee, together with the members or officers of such other bodies within the Division that the Bureau may specify. The number of Titular Members shall not exceed ten unless otherwise determined by the Bureau.

[Continue unchanged to end of current text.]

New paragraph following current text: Additionally, a Division Committee may elect no more than six National Representatives on the nomination of Adhering Organizations, with no more than one representative from a given Adhering Organization. The term of a National Representative shall be two years, with the possibility of renomination and reelection consecutively for only two more years. Exceptional circumstances must be established and special permission obtained from the Bureau for the election of a National Representative from a country already represented on the Committee by a Titular or Associate Member.

The Bureau has already defined the additional members of the Division electorate for 2003 to be members of the Division's nominating committee who are not included above (usually three individuals); and chairmen of all active task groups in the Division, along with chairmen of task groups whose projects have been completed within the period 2000-2002.

Dr. Becker commented that the role of National Representatives on Division Committees was seen as being very important and noted that they are now part of the Division electorate, whereas the National Representatives to Commissions were not permitted to vote. National Representatives will also participate in the project approval process. Since NAOs will need to know the composition of the Division Committees before making nominations, the letter requesting nominations will be sent out after the General Assembly.

Prof. Leigh (UK) noted that the reduced electorate is a concern to the UK delegation and proposed an amendment to the proposed text of Bylaw 4.103:

The Titular members of each Division Committee shall be elected by the an electorate comprising the Titular Members, Associate Members and National Representatives on the Division Committee, together with the members of Division Commissions and task groups whose projects are in progress or have been completed during the current biennium. Division membership in this category should not be automatic but subject to the approval in each individual case by the Division President to ensure a balanced representation within the Division.

This amendment was seconded by Prof. Hegarty (Ireland). Dr. Becker noted that there are technical issues with the proposed amendment. The amendment uses terms that are not defined in the Bylaws, such as project task group. The amendment would also allow each Division to set its own electorate. The Bureau sought to maintain uniformity. Dr. Becker was asked to describe the system for choosing AMs and NRs. He noted that the system is based on the current Bylaws and it is intended to ensure an equitable geographic distribution of members of IUPAC bodies.

Prof. Wilson (US) commented that all the Division Presidents are greatly concerned about the dramatic decrease in the size of the electorate. He proposed that the original motion be adopted with a recommendation that the problem be addressed. Prof. Berek (Slovakia) asked why the number of NRs on Division Committees was limited to six. Dr. Becker replied that this was done to maintain the Committees at an optimum size for conducting their business. The number six was selected to match the number of Associate Members.

Prof. Collins (Brazil) noted that the CCE would have an unlimited number of National Representatives. She suggested that Division Committees should have more NRs or a contact person from each NAO. Dr. Becker replied that it might be a good idea to have such designated contacts for each Division at each NAO in order to facilitate identification of representatives on task groups.

Prof. Cvitaš (Croatia) asked why only Task Group Chairmen were part of the electorate and not all task group members. Dr. Becker replied that the membership of Task Groups was sometimes not well defined.

Prof. Leigh requested a serious undertaking from the Officers to consider this issue further. With the approval of the seconder, he then withdrew the proposed amendment. Dr. Hayes put the question; voting was by cards; the motion was declared to have passed with no need for a formal count.

APPENDIX V

IUPAC DIVISION VIII

Division of Chemical Nomenclature and Structure Representation

Advisory Subcommittee Terms of Reference

1. To advise the Division Committee on the needs of the chemistry community with respect to standard systems for designating chemical structures, including both conventional nomenclature and computer-based systems.
2. To propose and participate in projects for the Division, and to advise on project leaders and other suitable participants.
3. The Committee will not meet in full on a regular basis; the Division Officers will authorise meetings of subgroups as needed to address specific issues, and will call larger meetings when it seems necessary to consider major issues of general interest. Otherwise, discussions will take place via an e-mail listserver.

APPENDIX VI**IUPAC DIVISION VIII****Division of Systematic Nomenclature and Structure Representation****Advisory Subcommittee composition (as of 01/26/02)**

Dr Hidetsugu Abe (Toyohashi U of Technology)
Professor Steven M Bachrach (Trinity U San Antonio, USA; Editor-in-Chief, Internet Journal of Chemistry)
Dr Byron J Bossenbroek (Columbus, OH, USA)
Mr Jonathan Brecher (CambridgeSoft, USA)
Dr John Brennan (European Patent Office, Netherlands)
Professor Neil G Connelly (Bristol, UK)
Professor Richard Cammack (Kings, London, UK; Chairman IUPAC-IUBMB Joint Commission on Biochemical Nomenclature)
Professor Franco Cozzi (U Milan, Italy)
Dr Ture Damhus (Novozymes, Denmark)
Professor Andreas Dress (Bielefeld, Germany)
Professor Andrey Erin (ACDLabs, Russia)
Dr Geoff Fairhurst (BASF, Germany)
Professor Henri A Favre (Montreal, Canada)
Dr Patton M Giles (CAS, ACS Nomenclature Committee)
Dr Jonathan M Goodman (Unilever Centre for Molecular Informatics, Cambridge, UK)
Professor Richard M Hartshorn (U Canterbury, New Zealand)
Dr Karl-Heinz Hellwich (Frankfurt, Germany)
Professor Bernardo J Herold (Lisbon, Portugal)
Dr Alan T Hutton (Cape Town, South Africa)
Dr Wolf-Dietrich Ihlenfeldt (Computer Chem Center, U of Erlangen-Nurnberg, Germany)
Professor Aubrey D Jenkins (Sussex, UK)
Professor Jaroslav Kahovec (Prague, Czech Republic)
Professor 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)
Professor Ebbe Nordlander (Lund, Sweden)
Professor Vincent L Pecoraro (Michigan, USA; Associate Editor, Inorg Chem)
Professor C Dale Poulter (Utah, USA; Editor, J Org Chem)
Professor Damon D Ridley (U of Sidney, Australia)
Dr Steve Stein (NIST, 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 Institute of Organic Chemistry, China)

APPENDIX VII

Responses from Steve Heller (SH) and Steve Stein (SS) to the questions about the IUPAC Chemical Identifier project raised at the IUPAC Division VIII Committee meeting on January 26th 2002:

S. Heller: As for the questions from last Saturday, I believe I did answer them more or less correctly at that time, but perhaps not fully enough for all. So here is a more detailed set of answers.

S. Heller: If you specify a tautomer, then you get the "name" for that tautomer. If you turn on the tautomer switch you get the "name" for "all" tautomers, no matter how you have drawn the structure. (I.e., the program does use the single/double bond positions in creating the "name").

S. Stein: Stated differently, if a structure is perceived to have tautomeric isomers (according to a specific set of rules), the IChI generator will generate a separate, clearly labelled tautomer identifier (all of its tautomers will generate the same IChI tautomer name). It is up to the user whether or not he wishes to use this descriptor. The exact species will always get a specific exact name, regardless of whether or not it is a tautomer.

S. Heller: Yes, there is an indication every time coordinates are invoked during a structure analysis (e.g., when checking for cis/trans).

S. Stein: All perceived stereochemistry will be labelled.

S. Heller: The program does go from structure to IChI name and vice versa, but from an IChI name you get only the 2D connection table, not the structure (unless there are x,y coordinates provided).

S. Stein: The IChI stores the *normalized* structure as a connection table, therefore the IChI can only regenerate the information after normalization. We are still debating whether auxiliary information (coordinates, positions or charges and double bonds, etc) should be stored along with the IChI.

S. Heller: Lastly, the atomic coordinates for stereochemical drawing are important only if they effect the parity (see item 8.3).

1 February 2002

APPENDIX VIII

Representation of Structural Formulas used in the Mineral Powder Diffraction File

Prof. S. C. Abrahams
Chairman, IUCr Commission on Crystallographic Nomenclature
Southern Oregon University
Physics Department
1250 Siskiyou Blvd
Ashland, OR 97520
USA

Dear Sidney,

The (new) IUPAC Division of Chemical Nomenclature and Structure Representation (Division VIII) has received a request from Professor Peter Bayliss that IUPAC should recognise the scheme for representation of structural formulae used in the Mineral Powder Diffraction File. The scheme is described in *American Mineralogist*, 1998, 83, 126-132. I should be grateful for any background information you might be able to give me on this, specifically:

- whether the scheme is regarded as acceptable by IUCr
- who would be a useful IUCr contact for discussion of this request
- other suggestions for suitable reviewers in this area

With thanks for any help you can offer, and personal best wishes for the coming year.

Sincerely
Alan McNaught
(President, IUPAC Division VIII)

From: S. C. Abrahams [SMTP:sca@mind.net] <mailto:[SMTP:sca@mind.net]>
Sent: Sunday 6 January 2002 17:17
To: Alan McNaught
Subject: RE: General and Structure-type Formulas for Minerals etc.

Dear Alan:

It was a pleasure to hear from you on Friday, giving me the opportunity of congratulating you on your recent election as chair of the new IUPAC Division.

Responding to your enquiry about the scheme for representing structural formulas proposed in the *American Mineralogist*, 1998, 83, 126-132, the authors have not approached the Commission on Crystallographic Nomenclature for IUCr recognition, hence we have no 'official' position on these proposals. However, I have now obtained a copy and, at first reading, receive the impression that the scheme is specifically designed for use in the International Center for

Diffraction Data (ICDD) Powder Diffraction File. This is the primary source of such data for all users.

Initially, the appropriate IUCr contact for an impression of the value/importance of the proposals is probably the Commission for Powder Diffraction, with Prof. Paolo Scardi as chair. He may be contacted at: Paolo.Scardi@ing.unitn.it <mailto:Paolo.Scardi@ing.unitn.it>

Other suggestions for suitable reviewers in this area are:

Sturges Bailey, U. Wisconsin, at bailey@geology.wisc.edu
<mailto:bailey@geology.wisc.edu>

Charles Prewitt, Carnegie Inst. Washington, at prewitt@gl.ciw.edu
<mailto:prewitt@gl.ciw.edu>

Simon Redfern, U. Cambridge, at satr@esc.cam.ac.uk
<mailto:satr@esc.cam.ac.uk>

Please do not hesitate to let me know if I can be of further help.

With all best wishes.

Sidney

APPENDIX IX

**IUPAC****CAS/IUPAC Conference on Chemical Identifiers and XML for
Chemistry
PRELIMINARY ANNOUNCEMENT****The Pfahl Executive Education and Conference Center and The Blackwell
at The Ohio State University, Columbus, Ohio, USA
July 1, 2002**

This conference will bring together experts to survey current activities in the research and development of chemical substance representations and identifiers, including both nomenclature and computer-based structural descriptions, and of chemical markup language.

The conference is designed for researchers and developers working in the areas of chemical identifiers and chemical markup language and chemical information specialists, database producers, and others who have an interest in or utilize chemical substance information.

Speakers for the conference include:

- Jonathan Brecher (CambridgeSoft Corporation): From chemical name to structure: finding a noodle in the haystack
- Alexander Lawson (MDL Information Systems GmbH): Nomenclature practice and post-Postman factors
- Peter Murray-Rust (Department of Pharmaceutical Sciences, University of Nottingham): The chemical semantic web: a common infrastructure for chemistry
- Henry S. Rzepa (Department of Chemistry, Imperial College of Science): The vision of a chemical semantic web
- Stephen E. Stein (Physical and Chemical Properties Division, NIST): The IUPAC Chemical Identifier
- Matthew J. Toussant (CAS): CAS chemical identifier systems
- Antony J. Williams (Advanced Chemistry Development): Unifying chemical nomenclature standards
- The roundabout of names and structures

- Janusz L. Wisniewski (MDL Information Systems GmbH): Computer-based naming service for very large chemical databases: from AutoNom in the Beilstein File to AutoNom in the ISIS system

The conference is being organized by David W. Weisgerber, CAS (retired).

The conference will begin with a welcoming reception on the Sunday evening preceding the meeting. The one-day conference will be held in the Pfahl Executive Conference Center on The Ohio State University campus and conclude with a banquet on Monday evening. An optional visit to Chemical Abstracts Service will be offered to the attendees on Tuesday morning, July 2, 2002. Hotel accommodations will be provided by The Blackwell, a new upscale hotel located adjacent to the Pfahl Executive Conference Center. Information will be posted on the CAS and IUPAC websites.

APPENDIX X

Review of Documents: The Role of Divisions and of IDCNS

Many IUPAC projects (perhaps most of them) result in a publishable document – a Technical Report or a Recommendation. To maintain IUPAC's credibility, it is important that each document be technically correct and that it be as consistent as possible with previous pronouncements by the Union. The cognizant Division(s) [or occasionally Standing Committee] has the primary responsibility for the content, but the Interdivisional Committee on Nomenclature and Symbols [IDCNS] has long played a key role in providing quality assurance on an IUPAC-wide basis. Indeed, the Bureau has largely delegated to IDCNS its statutory authority to approve "recommendations for international agreement in nomenclature, symbols, terminology and conventions." This system has generally worked very well, but there are some continuing problem areas in the operation and timeframe for IDCNS review. Moreover, with the elimination of Commissions as an intermediate level of review, there is a need to assure that future documents are adequately reviewed before approval by the Division. Specifically, the following concerns should be addressed:

1. There is no consistent policy or procedure for review and approval of documents within Divisions. The Division President's approval is based on whatever criteria he believes are appropriate. His signature is accepted by IDCNS as attesting to the technical quality of the document.
2. *Technical Reports* are currently reviewed only by the Officers of IDCNS, and the review is largely for consistency with previous work, particularly with respect to chemical nomenclature and presentation of symbols and units. The Officers are sometimes overloaded with documents, and completion of the review can be seriously delayed.
3. *Recommendations* are reviewed by the Officers, as above, but are also reviewed by a number of Division representatives to IDCNS. In addition, Provisional Recommendations are subject to a statutory five-month public comment period. This process is extremely valuable, but it often causes significant delays in final approval and publication.
4. Most of the documents reviewed deal with *terminology*, not *nomenclature* [which is used by IUPAC to refer to the naming of chemical substances]; yet the name of IDCNS does not reflect this broader responsibility.

After discussions with a number of people, including Officers and former Officers of IDCNS, I have prepared these guidelines for the review and approval process and for a restructuring and renaming of IDCNS. The Bureau has endorsed the guidelines in general, but details can certainly be changed if necessary.

Point (4) above can be handled most easily:

- Following formal approval by the Executive Committee, our central review group will be called the *Interdivisional Committee on Terminology, Nomenclature and Symbols*, with the abbreviation *ICTNS*. The abbreviation is very close to the present IDCNS, but has the desirable feature of using *I*, not *ID*, to represent the single word *Interdivisional*.

The problem in Point (2) will be addressed as follows:

- The central “core” membership of ICTNS will consist of a Chairman, Secretary and at least two additional Titular Members who are able and willing to review Technical Reports. Tom Cvitas, who is expert in physicochemical symbols and units, will remain as Chairman. Bernardo Herold, an expert in chemical nomenclature, will become Secretary in place of Val Metanomski, who has asked to be relieved of the secretarial responsibilities. However, Val will continue to use his nomenclature expertise in the review of documents. Jack Lorimer, also expert in symbols, units, etc., will become a “core” TM and will be available for review of documents. One or more additional TMs may be added.
- I believe this augmentation of the core capability will help in obtaining timely and high quality reviews. However, I have been assured of further backup if needed from the new Chemical Nomenclature Division and from the re-established Commission on Physicochemical Symbols, Terminology and Units, which has IUPAC-wide responsibilities.
- To reduce further the workload on ICTNS, we plan to have the Secretariat handle such functions as non-technical editing, which have imposed unnecessary burdens on the Committee’s Officers.

In order to address the potential problems raised in Point (1), we must require that each Division establish adequate review procedures, which must be better integrated with ICTNS, as follows:

- Since documents vary greatly in their purpose, type, length, etc., I think we should not be overly prescriptive regarding the nature of the Division review. [For Recommendations there are specific requirements about outside consultation, which will remain in effect.] In many instances the task group chairman will have conducted an extensive review by seeking and acting on comments on draft documents; in other cases, a document may be largely the product of one or two individuals who have had little outside interaction. The Division President, Division project coordinator and/or other members of the Division Committee should know enough about the project to be able to judge what additional refereeing is necessary.
- I do not want to add an additional layer of technical review beyond the Division, since it would require more effort and time. However, I think it is important that ICTNS be sure that such review has been carried out well, and this can probably best be done through the Division representative to ICTNS. As in the past, each Division will nominate one Titular Member to ICTNS. This individual should be familiar with the Division’s program and must be delegated the authority within the Division to coordinate review of all documents. He/she is not expected to be expert in all fields or necessarily to carry out a personal review, but rather to ensure and certify to ICTNS that the review has been adequate. In the past, the Division representative to IDCNS has been selected on the basis of his interest in nomenclature, symbols, etc. and ability to contribute to reviews of Recommendations. Those qualifications are still desirable but probably less important with the increased core capability of ICTNS. What we are asking now is that the Division representative have the stature within the Division to see that reviews of documents are carried out carefully and promptly. Ideally, this representative will be also a Titular Member of the Division Committee. I realize that in some instances it may not be feasible to identify a Division Committee TM who also has the ability, interest and willingness to take on the task of review coordinator. If that is the case, please be sure that the Division representative has adequate “clout” to get the

job done and that he/she has an opportunity to meet occasionally with the Division Committee and become a part of the Division management.

- There will no longer be a set of Associate Members on ICTNS nominated by each Division. However, there is provision for a small number of AMs, to be selected individually, primarily to bring in additional expertise and to help ensure continuity of expertise as the membership of the Committee changes. Suggestions for individual AMs are welcomed. Such suggestions should be sent to the Officers of ICTNS or submitted through the Secretariat and will be considered by the President.
- ICTNS will meet at the General Assembly, as do all Standing Committees. However, with increased use of e-mail, the routine “even year” meeting held in the past is not felt to be essential. Funds previously allocated to that meeting will be used to expand the Titular Membership, as described above; to permit some AMs to participate in the meeting at the GA; and to allow smaller meetings of Officers or specific groups as required.

In order to address Point (3) above, new procedures for handling Recommendations have been developed by IDCNS for implementation in 2002. Some aspects need modification in order to comply with the requirements of Bylaw 2.11, which requires a five-month public comment period. However, we believe that some actions can be handled concurrently in order to accelerate the process while remaining in compliance with the Bylaw. That will be the subject of a separate communication.

APPENDIX XI

Nomenclature World Wide Web Database – Statistics

Statistics based on log of IP addresses used each day. Total usage to date 1080000. Data on 163 countries recorded so far and summary data for 1996-2000 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	max
Total usage	296	650	1476	2786	5515	9813	14493
Search Facility	-	-	-	204	1663	4169	6897
Bibliographic Data	-	61	142	235	325	470	641
Map of Usage	-	7	8	29	37	58	103

IUBMB Nomenclature

Enzymes	16	54	124	320	1086	2088	3212
EC 1	-	-	-	35	241	487	855
EC 2	-	-	-	-	180	438	737
EC 3	-	-	-	-	165	427	878
EC 3.4 (50 file)	-	-	-	200	285	281	259
EC 3.4 (single)	-	-	-	-	-	134	324
EC 3.4 (total)	-	-	-	-	-	336	505
EC 4	-	-	-	-	90	223	437
EC 5	-	-	-	-	64	164	358
EC 6	-	-	-	-	46	138	300
reaction	-	-	-	-	48	119	221
newenz	-	-	-	-	53	60	102
Enzyme Supplement 5	-	-	42	66	79	53	75
Enzyme Kinetics	-	-	16	61	152	249	434
Biochemical Thermodynamics	-	-	22	40	66	107	216
Electron Transport Proteins	-	-	-	-	58	107	188
Isoenzymes	-	-	14	28	68	106	231
Incomplete Nuc. Acid Sequence	-	9	20	31	50	75	103
<i>myo</i> -inositol	-	-	11	23	43	74	111
Branched Chain Nucleic Acids	-	3	6	10	40	63	159
Peptide Hormones	-	-	-	-	32	51	79
Multienzymes	-	-	10	13	18	25	39
Translation Factors	-	-	-	-	11	18	34

Year	1996	1997	1998	1999	2000	2001	max
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Both Committees

Committees' Homepage	18	38	65	123	268	423	592
Newsletter	-	-	25	59	145	304	630

IUPAC/IUBMB Nomenclature

Carbohydrates	46	72	144	237	453	835	1160
Steroids	12	21	87	93	396	811	1245
Amino Acids & Peptides	31	62	135	186	359	670	1076
Folic acid	-	-	-	60	58	210	213
Vitamin B-6	-	-	-	34	95	155	245
Vitamin B-12	-	-	-	49	69	146	260
Nucleic Acid Abbreviations	-	-	-	45	77	136	226
Glycoproteins	-	-	20	32	71	134	234
Lipids	-	-	-	29	70	132	220
Tetrapyrroles	-	-	-	-	-	124	226
Cyclitols	-	-	21	51	72	113	160
Polypeptide Conformation	-	8	14	34	61	111	229
Biochemical Phosphorus	-	-	-	-	62	103	254
Glycolipids	-	-	15	35	65	91	156
Carotenoids	-	-	-	-	46	84	160
Polysaccharide Conformation	-	8	14	26	49	82	151
Tocopherol	-	-	21	33	48	80	123
Lignans and Neolignans	-	-	-	-	-	71	118
Retinoids	-	-	-	-	35	71	104
Vitamin D	-	-	-	-	47	69	112
Polynucleotide Conformation	-	7	15	27	44	68	97
Polymerised Peptides	-	-	-	-	34	56	104
Prenols	-	-	-	19	33	55	98
Quinones with Isoprenoid Chain-	-	-	-	-	-	47	82

IUPAC Nomenclature

Class Names Glossary	138	157	430	693	1039	1504	2249
Physical Org Chem Glossary	29	36	136	343	751	1089	1811
Atomic Weight	23	48	95	144	310	651	1199
Stereochemical Glossary	-	32	85	135	231	392	767
Bioinorganic Glossary	-	-	61	108	201	391	719
Section F (Natural Products)	-	-	-	14	121	321	478
Medicinal Chemistry Glossary	-	-	56	87	150	316	524
Periodic Table	-	-	-	17	155	291	522
Fused Ring	-	-	64	73	110	198	288
Ions and Radicals	-	-	-	-	72	150	256
Gold Book	-	-	-	-	80	127	185

	1996	1997	1998	1999	2000	2001	max
von Baeyer	-	-	-	29	61	106	152
Numerical Term	-	18	27	35	54	99	169
Spiro	-	-	-	26	47	90	121
Hantzsch Widman	12	14	31	46	56	89	122
Delta Convention	8	9	19	30	54	82	142
Phanes	-	-	31	42	56	80	118
Element Name > 100	-	-	-	20	45	78	169
Section H (Isotopic Label)	-	-	26	34	46	73	125
Lambda Convention	6	8	17	28	40	60	86
Guide Errata	-	-	-	20	21	25	37

GPM
11 January 200