

IUPAC DIVISION (VIII) OF CHEMICAL NOMENCLATURE AND STRUCTURE REPRESENTATION

Report to IUPAC Bureau and Council, August 2003

I. Highlights

- I.1 IUPAC Chemical Identifier.** Good progress and prospects for acceptance by the community, including articles in *Nature* and *Chemical & Engineering News* (items II.4.1; IV.6 and 7)
- I.2 Organic Preferred Names.** New Blue Book draft completed, including recommendations for selecting Preferred IUPAC Names (PINs), now undergoing expert review (item II.3.2)
- I.3 Revised Red Book.** New draft completed and under expert review (item II.3.5)
- I.4 Reconstitution of the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature.** JCBN reconstituted as a smaller Commission with facilities for project-based activities as well as ongoing input to the Enzyme List (item III)
- I.5 Project development.** The lack of input from the community, and the need for studies of requirements and feasibility (item II.4)

II. Report of activities 2002-2003

- II.1 Context.** The work of the Division of Chemical Nomenclature and Structure Representation is concerned entirely with standards for the transmission of chemical information, and as such addresses the following long-range IUPAC goals:
- b) IUPAC will facilitate the advancement of research in the chemical sciences through the tools that it provides for international standardization and scientific discussion.*
- d) IUPAC will foster communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries.*
- II.2 Establishment of the new Division.** Established in January 2002, the new IUPAC Division VIII consists of a Division Committee (twelve members and six National Representatives) and an Advisory Subcommittee (45 people). The Joint IUPAC-IUBMB Commission on Biochemical Nomenclature reports to the Division Committee. Division members have access to a Web Discussion Board, on which minutes of meetings and current draft recommendations are posted for comment.

II.3 Current projects

II.4.1 IUPAC Chemical Identifier.

A prototype algorithm for well-defined, discrete covalent organic structures was distributed for testing in March 2002. The project group reviewed feedback at a meeting in Columbus on June 30th; no problems were apparent. This first version of the program deals with covalently bonded structures only, with options to specify tautomers, stereochemistry and isotopic substitution, and uses .mol files as input. A second version, expected to be available in mid-2003, will extend the range of applicability to include inorganic and organometallic

structures. A meeting of the project team and other interested parties will take place at NIST in November, to receive feedback from testing of this second release, and to define the way forward. Consideration will be given to a further extension of the program to include polymers, and to ways of encouraging use of the new identifier.

A CAS/IUPAC Conference on Chemical Identifiers and XML for Chemistry was held in Columbus on July 1st 2002. This meeting was devised following discussions with *Chemical Abstracts* staff when the IUPAC Chemical Identifier project was initiated. The speakers reviewed various types of identifier, and explored their relationship with potential XML schemas for molecular data. The conference abstracts are available at:

<http://www.rsc.org/IUPAC8/attachments/CAS-IUPACConf.doc>

II.3.2 Organic Preferred IUPAC Names (PINs)

Work on the new Nomenclature of Organic Chemistry (IUPAC Blue Book), including recommendations for identifying IUPAC-preferred names, is approaching completion. A complete draft (more than 1000 pages) is posted for review on the Division VIII web board. Publication is expected in late 2004.

II.3.3 Corrections to Revised Nomenclature of Organic Chemistry Section F: Natural Products

A number of errors and inconsistencies in this document have been pointed out and a small Division VIII group met in Boston in August 2002 to consider how to proceed. It is likely that a Corrections and Modifications document will be published both in print and on the web.

II.3.4 Alignment of Organic and Inorganic Preferred Names

Principles for rationalising naming recommendations in areas of overlap were discussed at meetings in Cambridge, UK, in September 2001 and January 2002, and decisions were made on how to proceed with the revision of the Red Book (Nomenclature of Inorganic Chemistry) and the new Blue Book (Nomenclature of Organic Chemistry). The new Red Book will not attempt to assign preferred names; this exercise will be left for a subsequent project. Proposed guidelines for dealing with organometallic compounds have been favourably received by the Alignment Project Group.

II.3.5 Revision of “Nomenclature of Inorganic Chemistry”

Revision of the IUPAC Red Book is approaching completion; a review draft has been posted on the IUPAC Division VIII web board. Publication in 2004 is expected.

II.3.6 Rotaxanes

A first draft of recommendations for naming discrete (as opposed to macromolecular) rotaxanes has been prepared and is being reviewed by the project team.

II.3.7 Fullerene nomenclature Part II

This extension of the recently published Part I recommendations to larger and more complicated molecules is approaching completion

Macromolecular Nomenclature Projects

The following projects have been carried over from the Macromolecular Nomenclature Commission, and are continued in full cooperation with Division IV's Subcommittee on Macromolecular Terminology:

II.3.8 Structure-based nomenclature for cyclic macromolecules

II.3.9 Nomenclature for macromolecular rotaxanes

II.3.10 Nomenclature of dendrimers and hyperbranched oligomers and polymers

II.3.11 Process-based nomenclature for chemically modified polymers

All are due for completion in 2003, and new drafts have been reviewed at this IUPAC General Assembly.

II.4 Scoping exercises

Since its inception in January 2001, the new Division has received no unsolicited project proposals from the community. It seems clear that the responsibility for developing proposals will rest with the Division Committee, and the Division has therefore been carrying scoping exercises to establish needs and feasibility.

II.4.1 Stereochemistry

Requirements for future development of stereochemical nomenclature in all disciplines are being reviewed, and a scoping exercise was carried out during 2002. This has yielded a project proposal for a IUPAC book on this subject, which is now being assessed.

II.4.2 Structure representation

A scoping exercise on the need for standard structure-drawing conventions, with particular reference to on-screen representation, is being carried out, aided by input from a very active web-based discussion facility. A report is under consideration by the Division Committee and will probably lead to a project for defining IUPAC guidelines.

II.4.3 Inorganic nomenclature projects

A Division VIII working group met in Cambridge in April 2003 to develop plans for work in this area. The group is attempting to define projects on the following subjects, among others, and to identify suitable participants.

- boron nomenclature
- organometallic stereochemistry
- preferred IUPAC names for inorganic and organometallic compounds
- nomenclature of metallacycles

- stereodescriptors for complexes of seven-coordination and more

II.5 Joint IUPAC-IUBMB Commission on Biochemical Nomenclature (JCBN)

Joint activities of the two Unions are channelled through this Joint Commission, which has been reconstituted in the light of the changes in arrangements for managing IUPAC's work (see section III). The main activities of the Commission are

II.5.1 Maintenance and updating of the Enzyme List

This is a very substantial and continuous operation drawing on advice from IUPAC participants on chemical names for substrates, reagents and products

II.5.2 Maintenance and development of specialised naming systems for natural products

Classes of natural product of interest to biochemists, especially steroids, amino acids and peptides, carbohydrates, lipids and nucleic acids require local specialised systems for naming. A project to review and update carbohydrate nomenclature is being assembled.

II.5.3 Advice for biochemists on names for specific compounds of biochemical importance

The development of a synonyms database for compounds in common biochemical usage is under consideration, building on work in progress at the European Bioinformatics Institute and at the University of Missouri.

III. Reconstitution of the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature

- III.1*** Future arrangements for joint IUPAC-IUBMB nomenclature activities were considered by the IUPAC Bureau in September 2002, and a three-person working group was appointed to open discussions with IUBMB. This group, consisting of IUPAC's Executive Director (John Jost) and Secretary General (Ted Becker) and myself, made contact with IUBMB Officers by e-mail, and discussions took place with the IUBMB Secretary General (Jacques-Henri Weil), President (Brian Clark), Treasurer (Brian Beechey), and Publications Committee Chairman (Angelo Azzi), during January-March 2003. Richard Cammack (Chairman of JCBN) was involved during final discussions over new terms of reference.
- III.2*** It became clear very soon that IUBMB wished to maintain NC-IUBMB as an entity separate from any joint body. This being so, it was agreed that JCBN needed to continue in something like its present form. However, IUPAC wished to modify funding arrangements so as to be able to assign more money directly to approved projects and less to "operational" matters (e.g. annual meetings of the full Commission). It was therefore agreed that, instead of eight Titular Members (four from each Union) and eight Associates, the Commission should consist in future of four titular Members (two from each Union) and eight Associates. One of the Titular Members (appointed by IUBMB) would be the Chairman, and another (appointed by IUPAC) would be the Secretary. The Chairman would be an ex-officio member of the IUPAC Division VIII Committee, with participation funded by IUBMB.

- III.3** There would still be a need for an annual meeting, most conveniently held in conjunction with NC-IUBMB, for which only Titular Members would have guaranteed funding.
- III.4** As now, NC-IUBMB would be responsible for maintaining the Enzyme List, with advice from IUPAC members of JCBN on systematic naming etc.
- III.5** A mechanism for approval and management of projects was agreed. Under IUPAC's new project-based system, all projects are formulated as proposals for consideration by the appropriate Division Committee. Each Division has a biennial budget that can be assigned to approved projects, and some of the funding currently assigned by IUPAC to JCBN will be added to this, with the intention that the combined sum can be requisitioned for suitable projects over the whole range of chemical nomenclature, including projects arising from JCBN. JCBN projects will be funded jointly by the two Unions, and a mechanism for requesting corresponding funds from IUBMB was agreed.
- III.6** Terms of reference for the new JCBN are attached, and will take effect from January 1st 2004.

IV. Division VIII Publications

Since January 2002, the following nomenclature publications have appeared:

- IV.1** Fullerenes, Part I (inherited from Commission III.1 on Nomenclature of Organic Chemistry)
<http://www.iupac.org/publications/pac/2002/7404/7404x0629.html>
- IV.2** Phanes, Part II (inherited from Commission III.1 on Nomenclature of Organic Chemistry)
<http://www.iupac.org/publications/pac/2002/7405/7405x0809.html>
- IV.3** *Chemistry International* article on the birth of the Division
http://www.iupac.org/publications/ci/2002/2402/news_chemical.html
- IV.4** *The Alchemist* article: "What's in a Name"
<http://www.chemweb.com/alchem/articles/1015947151360.html>
- IV.5** *The Alchemist* article: "That IChI Feeling"
<http://www.chemweb.com/alchem/articles/1015947904091.html>
- IV.6** *Nature* article: "Chemists synthesize a single naming system"
<http://www.rsc.org/IUPAC8/attachments/IChI-Nature502.pdf>
- IV.7** *Chemical & Engineering News* article: "Unique Labels for Compounds"
<http://pubs.acs.org/cen/today/nov26.html>
- IV.8** Article on Phane Nomenclature by Henri Favre and Warren Powell in "Cyclophane Chemistry for the 21st Century" (Research Signpost, 2002)

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August 2003

IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN)

Terms of Reference (March 2003)

Responsibilities

- 1.0 To maintain and develop naming systems for classes of natural product of interest to biochemists, especially steroids, amino acids and peptides, carbohydrates, lipids and nucleic acids.
- 2.0 To maintain and develop standards for symbolism to be used in databases for biopolymers.
- 3.0 To provide advice for biochemists on chemical names for compounds of biochemical importance.
- 4.0 To ensure that all recommendations are compatible with those issued by other nomenclature bodies of IUBMB and IUPAC.

Procedures

- 1.0 The Commission considers project proposals for work to be carried out under its own auspices, and forwards supported proposals to the IUPAC Secretariat and to the Chairman of IUBMB's Committee on Publications. Project review by IUPAC follows standard IUPAC procedures, involving assessment by external referees and by the appropriate Division Committee [normally the Division (VIII) of Chemical Nomenclature and Structure Representation]. Copies of all reviews obtained are sent to IUBMB, and agreement on approval and on level and distribution of funding is obtained by correspondence between IUBMB (via the Publications Committee Chairman) and the IUPAC Division VIII President. Approved projects are managed by the Commission.
- 2.0 Before recommending any resulting material for publication as an IUBMB-IUPAC document, the Commission should ensure that the fullest possible consultations have taken place and the widest possible consensus has been reached with the appropriate bodies of each Union: for IUPAC, the Division (VIII) of Chemical Nomenclature and Structure Representation and the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS); for IUBMB, the Nomenclature Committee (NC-IUBMB).
- 3.0 Approval to publish any material as an IUBMB-IUPAC document is to be obtained in the case of IUPAC from the IUPAC Division VIII Officers and ITCNS, and in the case of IUBMB from the Executive Committee of IUBMB.
- 4.0 The Commission normally holds an annual meeting concurrently with that of NC-IUBMB, and with the approval of the President of the IUPAC Division of Chemical Nomenclature and Structure Representation and the Executive Committee of IUBMB.
- 5.0 Associate Members will receive all documents of the Commission and their opinion will be sought by correspondence. An Associate Member may attend any meeting of the Commission, but his or her expenses will not be defrayed by the respective Executive Committee unless he or she has been invited as an observer under item 6.0.
- 6.0 The Commission is entitled to invite observers from similar bodies and experts in special fields to attend the meeting. The IUPAC Division President or the IUBMB Executive Committee should be asked in advance to defray any expenses that would arise from such an invitation.

Composition and Terms of Office

- 1.0 The IUBMB-IUPAC Joint Commission on Biochemical Nomenclature is composed of four Titular Members, two appointed by IUPAC (including the Secretary) and two by IUBMB (including the Chairman), and up to eight Associate Members (appointed by JCBN itself).

- 2.0 The Chairman and the Secretary are each appointed for four years by the President of the appropriate Union, subject to whatever ratification is imposed by Union Statutes and Bylaws. JCBN may propose names of persons suitably qualified for appointment. The Chairman is ex officio a member of the IUPAC Division VIII Committee (Chemical Nomenclature and Structure Representation), with attendance at Division Committee meetings funded by IUBMB.
- 3.0 Candidates for Titular Membership may be proposed by the Commission. The Titular Members appointed by IUBMB shall also be Members of the Nomenclature Committee of IUBMB (NC-IUBMB).
- 4.0 The periods of service of the Titular Members and of the Associate Members are in accord with the Statutes and Bylaws of the appointing Union. The sum of the years of service as a Titular Member and as the Chairman or the Secretary must not exceed ten years.

