

Item 14.1 Proposed Division of Systematic Nomenclature and Structure Representation

The Executive Committee recommends to the Bureau and Council that a new IUPAC Division be established to centralize the Union's work on systematic chemical nomenclature, including computer-based structural representations. The EC has carefully examined alternatives for IUPAC's future in chemical nomenclature and concluded unanimously that this is a prudent move.

IUPAC's Role in Systematic Chemical Nomenclature. "Nomenclature" in IUPAC means many things – most of it more properly called "terminology". Each sub-field – spectroscopy, electrochemistry, photochemistry, combinatorial chemistry, etc. – has specialized terminology. None of this is being addressed here. What we are concerned with is the systematic nomenclature that has been and is being developed for chemical substances. Since 1919 this work has been among IUPAC's most visible efforts. It has been and until the end of this year will be conducted in three IUPAC Commissions [Nomenclature of Inorganic Chemistry (II.2), Nomenclature of Organic Chemistry (III.1), Macromolecular Nomenclature (IV.1)] and in the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN). Over the decades these bodies have made very significant contributions in laying the foundation for systematic nomenclature, but in recent years there has been increasing criticism of the ability of IUPAC to provide timely recommendations. The fragmentation of the separate Commissions has made it difficult to address interdisciplinary questions, and IUPAC has not been seen as a major player in the increasingly important field of computer-based nomenclature.

At Berlin, one of the major concerns in discontinuing Commissions was providing for continuation of work on this intricate system of nomenclature. After the General Assembly, the Secretary General was asked to investigate alternatives and did so via a Strategy Roundtable on *Representations of Molecular Structure: Nomenclature and Its Alternatives*, co-organized and chaired by Dr. Alan McNaught. All indications are that the Roundtable was very successful and represented a turning point for IUPAC's efforts in nomenclature. There were three principal reasons for the success: (1) The Roundtable was organized around asking potential "customers" what IUPAC should be doing. Participants included patent attorneys, industrial representatives, officials in international trade, journal editors and publishers, database providers, software experts, health and safety representatives, as well as interested and knowledgeable chemists and nomenclature experts. (2) A year before the Roundtable, Alan McNaught and Jean Claude Richer had prepared a document arguing for the need to emphasize computer representations of nomenclature and to coordinate the work of the then four separate nomenclature commissions. With the restructuring underway in IUPAC, this provided a guidepost to ways of integrating the work formerly carried out by these commissions. (3) The participants developed a number of novel and important proposals and recommendations. Of particular interest was a proposal that was refined during the Roundtable to create a "chemical identifier" – a computer-readable string of characters that can be translated back and forth to molecular structures and, with existing commercial programs, to conventional systematic IUPAC names.

The EC agreed in March 2000 to set up, under Dr. McNaught's chairmanship, the *ad hoc* Committee on Chemical Identity and Nomenclature Systems [CCINS] in order to initiate the Chemical Identifier project with a small task group, to analyze the ongoing nomenclature work in the four Commissions, and to recommend to the EC how best to pursue systematic nomenclature work in the future.

Item 14.1 Proposed Division of Systematic Nomenclature and Structure Representation

Consideration of Organizational Options. The EC [Stellenbosch, March 2001] accepted the objectives for future IUPAC efforts in chemical nomenclature, as given in the report by the CCINS, namely:

1. Identify the needs of the user community
2. Generate projects arising from those needs
3. Identify project leaders and task groups to carry out the work
4. Administer approved projects financially and monitor their progress
5. Evaluate existing projects, and ensure their continuity where appropriate
6. Ensure continued access to the expertise of current and past members of Nomenclature Commissions
7. Identify new sources of expertise and enable their involvement in IUPAC projects
8. Ensure 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 structure

The CCINS recommended the establishment of a *Division of Systematic Nomenclature and Structure Representation*, with overall responsibility for managing the maintenance and development of standard systems for designating chemical structures, including both conventional nomenclature and computer-based systems. The Division would be responsible for approving project proposals, on the basis of external review according to established IUPAC criteria, and for funding and monitoring approved projects. Funding would come from an established Divisional budget, or from the IUPAC Project Committee in exceptional circumstances.

The EC considered alternative organizational arrangements, including formation of an Operational Standing Committee or a continuation of the *ad hoc* CCINS, and took into account dissenting recommendations filed by two members of the CCINS. In the end, the EC concluded that the establishment of a Division to handle these matters would confer higher visibility and status on IUPAC's nomenclature work, which remains at the core of IUPAC activities, and would allow projects in this area to be administered and reviewed (through IDCNS) exactly as for the rest of the Union's scientific output.

The CCINS presented an operational plan for the new Division that includes the establishment of an Advisory Subcommittee of suitably experienced people to advise the Division Committee on the needs of the community, to initiate project proposals, and to suggest project leaders. The subcommittee, which will be formed only after consultation with the present Nomenclature Commissions and the other Division Committees, is viewed as essential, both to provide status for active members of existing Commissions, so that they can be persuaded to continue their involvement with IUPAC work, and to create momentum for work in this area. Periodically the other Division Committees and National Adhering Organizations will be asked to suggest new members for the Advisory Subcommittee.

The EC also accepted the CCINS observation that this arrangement could readily accommodate the IUPAC/IUBMB Joint Commission on Biochemical Nomenclature as a Commission attached to the Division. [See Item 14.2 for further details on JCBN.]

The EC also noted that the new Division will deal with *systematic* nomenclature for chemical compounds, not with all names of chemical substances. In particular, this Division will not be involved with the names of new elements. The Inorganic Chemistry Division should continue to

Item 14.1 Proposed Division of Systematic Nomenclature and Structure Representation

handle the authentication of the discovery of new elements and to appoint task groups as needed to recommend names for the elements.

The EC also expects continuing close scientific interactions between the new Division and other IUPAC Divisions, as indicated in its operational plan. For example, there is sometimes a close relation in polymers between systematic nomenclature and terminology, such as “block,” “ladder,” etc., which must be coordinated between Divisions.

Financial Considerations. Discussions in previous meetings of Council, Bureau and the three Divisions directly involved indicate strong support for the Union to continue its long-standing role in systematic chemical nomenclature and to be in the forefront of newer developments in computer-based approaches. The costs of IUPAC nomenclature work will depend largely on the scope of projects that the Union is able to support. However, it is also widely agreed that a continuing body will be needed to guide the program, ensure compatibility of nomenclature systems and provide for identifying project leaders and task groups with specialized expertise. From the fiscal standpoint, a Division Committee devoted to systematic nomenclature work will cost no more than another type of committee. The Treasurer has made plans in the budget for 2002-2003 to fund this Division, if approved, at a level comparable with the other Divisions.

Recommendation. The EC strongly recommends to the Bureau and Council that a new Division of Systematic Nomenclature and Structure Representation be established.

Terms of Reference

The Division of Systematic Nomenclature and Structure Representation 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.