

Dr R. M. Hartshorn

30 June, 2011

Report to IUPAC Council on Division VIII Activities

I am pleased to report that the Division of Chemical Nomenclature and Structure Representation is supporting numerous projects and activities in our area of responsibility – Nomenclature is a core IUPAC activity, and one which is clearly identified with IUPAC. Details on active projects, listed below, can be found at <http://iupac.org/indexes/Projects/bodies/800>. Apart from key project work and further development of the International Chemical Identifier (InChI) and Preferred IUPAC Names (PINs) a major new initiative in this biennium has been the development of closer contacts with organisations that are, or will be, users of nomenclature. New links with the International Standards Organisation (ISO) and the EU Commission on Taxation and Customs Union are examples of means by which nomenclature development and use can be enhanced.

The Sub-Committee on the IUPAC International Chemical Identifier (InChI) is the mechanism by which IUPAC maintains oversight of the scientific activities of the InChI Trust. It reports to Division VIII and to the Committee on Printed and Electronic Publications (CPEP). The Division also operates an Advisory Sub-Committee which we use as a way of extending links into our community of interest, particularly in relation to review of nomenclature proposals.

The area of nomenclature, perhaps more than others, needs to work hard to identify and nurture those with a spark of interest in the subject. Innovative suggestions and constructive comment on this issue are always particularly welcome.

Current Membership

Richard Hartshorn (President)

Gerry Moss (Past-President)

Ture Damhus (Secretary)

Titular Members:

Jonathan Brecher, Kirill Degtyarenko, Philip Hodge, Alan Hutton, Jeff Leigh, Jeffery Wilson, Andrey Yerin

Associate Members:

Karl-Heinz Hellwich, Jaroslav Kahovec, Ebbe Nordlander, József Nyitrai, Warren Powell, Jan Reedijk

National Representatives

Sundarababu Baskaran, Abdul Jalil Miah, Patrick Moyna, Hiroshi Ogino, Amélia Rauter, Ricardo Bicca de Alencastro

Division Elections

Election of officers and TMs for the 2012-13 biennium has been completed. This process took rather longer than planned, partly because of communication issues, but also because of the need to conduct officer elections after that for TMs. The Division VIII membership for the 2012-13 biennium that has been submitted to the IUPAC Council for approval includes:

Richard Hartshorn (President)

Karl-Heinz Hellwich (Vice-President)

Ture Damhus (Secretary)

Titular Members:

Andrey Yerin, Ebbe Nordlander, Warren Powell, Tony Williams, Amélia Rauter, Michael Beckett, Hinnerk Rey

Associate Members:

Alan Hutton, Jeffrey Wilson, Kirill Degtyarenko, Jan Reedijk, Nigel Wheatley, Phil Hodge

National Representatives:

Md. Abul Hashem, Wei Huang, Sundarababu Baskaran, Itrat Anis, Lupituko Luko M Kayula, Supawan Tantayanan, Vera Ahsen

Key Projects for 2010-2011

The new revision of the Blue Book has been in preparation for approximately 15 years. This massive task (currently ~1600 pages!) has been largely undertaken by Warren Powell and Henri Favre. The most recent draft was submitted to review by the Advisory Sub-Committee in the middle of last year. At the same time, an overall review was begun by a technical editor and the manuscript was submitted to ICTNS. A surprising amount of feedback was received. Some comments repeated concerns that had been considered and rejected in earlier review cycles, numerous minor errors were identified, as well as several new significant deficiencies. A few new controversies arose. The extent and tenor of some of these responses led us to suspend the technical editing and the ICTNS review, as it became clear that a further draft will be required. While it would have been desirable to achieve publication of this major book during IYC 2011, it is now clear that this will not happen.

The revision of Principles of Chemical Nomenclature, has been completed by Jeff Leigh and his team. At the time of writing this report, a complete set of proofs has been examined and submitted to the publishers (RSC). A set of final proofs has just been circulated, indexing will follow, and we anticipate that this book will be published well before the end of the year.

Project Reviews and New Funding Committed

Funding has been approved for eight new projects so far this biennium. These projects, together with the financial commitment from the Division (and from a co-funding body) are listed below.

2009-018-2-800 Recommendations on Nomenclature of Flavonoids

(<http://www.iupac.org/web/ins/2009-018-2-800>) USD 8,700 (Project Committee USD 8,700)

2009-040-2-800 InChI Requirements for Representation of Organometallic and Coordination

Compound Structures (<http://iupac.org/web/ins/2009-040-2-800>) USD 4,000 (Project Committee USD 4,000)

2009-041-1-800 InChI Requirements for Representation of Markush Structures

(<http://www.iupac.org/web/ins/2009-041-1-800>) USD 4,000 (InChI Trust USD 4,000)

2009-042-1-800 InChI Requirements for Representation of Polymers

(<http://www.iupac.org/web/ins/2009-042-1-800>) USD 4,000 (InChI Trust USD 4,000)

2009-043-2-800 Standard InChI-based Representation of Chemical reactions
(<http://iupac.org/web/ins/2009-043-2-800>) USD 5,000 (Project Committee USD 5,000)

2009-047-1-400 Definitions and Notations Relating to Stereochemical Aspects in Polymer Science
(<http://www.iupac.org/web/ins/2009-047-1-400>) USD 3,000 (Div IV USD 3,000)

2010-055-1-800 Basic Guidelines to the Nomenclature of Organic and Inorganic Chemistry
(<http://iupac.org/web/ins/2010-055-1-800>) USD 5,000

2009-022-2-800 Glossary of Small Molecules of Biological Interest
(<http://www.iupac.org/web/ins/2009-022-2-800>) USD 6,000 (Project Committee USD 6,000)

International Standards Organisation (ISO) Liaison

ISO has established a Technical Committee (TC 229) to examine aspects related to nanotechnology. Within that effort, a Joint Working Group (ISO TC 229/JWG 1) has been given the task of defining and establishing terminology and nomenclature standards for nanomaterials.

A Project Group (PG 11) has been set up within JWG 1 to identify priority areas for nomenclature development. Classes of molecules such as carbon nanotubes and metal clusters of various kinds are among those that have been identified. These are likely areas of nomenclature development collaboration between ISO and IUPAC.

ISO TC 229/JWG 1 met in Kuala Lumpur, Malaysia, from 6-10 December. Richard Hartshorn (Div VIII President) attended as the designated IUPAC liaison person, and the principal activity was to make a presentation on IUPAC activities and some relevant types of nomenclature that have already been established for other classes of compounds. A presentation was also made to JWG 1 on behalf of the International Council for Science (ICSU), of which IUPAC is a member, and which aims to ensure the integrity and scientific basis for vocabulary and definitions, and to promote harmonization of use across the scientific community.

The level of interest in the potential for collaboration between ISO and IUPAC on nomenclature activities can be judged from the reaction to the nomenclature presentation. It was originally scheduled to last 30-40 minutes, but ended up taking more than 2.5 hours due to the large number of questions and requests for more information on various aspects of IUPAC organization and activity, and on specific issues of nomenclature. Richard Hartshorn also attended their next meeting in St Petersburg, in May, to offer further advice on nomenclature issues.

An ISO Task Group, led by Andy Atkinson (Canada) and Martha Marrapese (USA), has been established to explore the potential relationships between ISO and IUPAC. At this stage a small group of representatives from IUPAC Divisions are being kept informed in order to engage further with the ISO Task Group when required. Those people are: Robert Loss (Div II), Sanjay Mathur (Div II), Javier Garcia-Martinez (Div II), Gerrit Koomen (Div III), Chris Ober (Div IV), Richard Jones (Div IV). This group, or a subset of it, will meet with Andy Atkinson and Martha Marrapese in San Juan.

The liaison between ISO and IUPAC has been established to explore possible collaboration on nomenclature development, but the goals of ICSU and the potential overlap with IUPAC interest in terminology means that it may be profitable to expand the scope of the ISO-IUPAC interaction to consider inclusion of aspects of terminology as well as nomenclature.

European Union Commission on Taxation and Customs Union

We have recently received a request from the EU Commission on Taxation and Customs Union for a training session on IUPAC Nomenclature. This group has been very interested in our recent

developments and current work, particularly related to InChI and Preferred IUPAC Names (PINs). This represents another real opportunity for closer engagement with nomenclature users

International Year of Chemistry

Division VIII activities that have the most visibility largely revolve around nomenclature – the development of nomenclature for new classes of compounds and dissemination and public engagement in relation to existing nomenclature recommendations. The major initiative for IYC 2011 will be publication of the revision of Principles of Chemical Nomenclature. As mentioned above, we are working towards publication of this book in time for the GA. A further project, 2010-055-1-800 Basic Guidelines to the Nomenclature of Organic and Inorganic Chemistry (<http://iupac.org/web/ins/2010-055-1-800>), is intended to provide a readily accessible guide to the essentials of chemical nomenclature. The documents will be concise and contain links and references to more detailed documents. We had hoped that the new Blue Book would be published this year, but that will not now be possible, for reasons detailed above.

Budget Report

The biennial budget allocation to Division VIII is USD 80,000. IUPAC guidelines are that approximately 70% (USD 56,000) of division budgets should be committed in support of project work, and the remaining 30% (USD 24,000) allocated to operational expenditure.

In Division VIII there has been a tendency to use somewhat more than the guideline amount of the budget for operational expenditure. This has continued as operational expenditure has been and will be used to support liaison activities (e.g. with the InChI Trust, ISO, ACS) that may lead to future projects. Operational expenditure from Division VIII is also used to support IUPAC involvement in the long-standing IUBMB-IUPAC Joint Commission on Biochemical Nomenclature.

At this point in the biennium project commitments (detailed above) of just under USD 40,000 have been made and operational expenditure has funded the off-year Division meeting (Lund, Sweden), and has contributed to the ACS-IUPAC Collaboration Summit, ISO Liaison, and InChI meetings.

Publications Related to Div VIII this Biennium

G.J. Leigh: Periodic Tables and IUPAC, *Chem. Int.* **31** (1) 4-6 (2009).

K.-H. Hellwich: *Chemische Nomenklatur – Die systematische Benennung organisch-chemischer Verbindungen* [Chemical nomenclature – the systematic naming of organic-chemical compounds] (3rd Ed., Govi-Verlag 2008).

Kemisk Ordbog [Chemical Dictionary] (3rd Ed., Eds. T. Damhus, S. Møller, A. Senning; Nyt Teknisk Forlag, 2008). A guide to the Danish adaption of IUPAC nomenclature recommended by the Danish Chemical Society.

Glossary of class names of polymers based on chemical structure and molecular architecture (IUPAC Recommendations 2009), M. Barón, K.-H. Hellwich, M. Hess, K. Horie, A.D. Jenkins, R.G. Jones, J. Kahovec, P. Kratochvíl, W.V. Metanowski, W. Mormann, R.F.T. Stepto, J. Vohlídal and E.S. Wilks, *Pure Appl. Chem.*, **81**(6), 1131–1186 (2009).

Karl-Heinz Hellwich, Elisabeth Weber: Glossar von auf der chemischen Struktur und der Molekülarchitektur beruhenden Polymerklassennamen, *Angew. Chem.* 2010, **122** (28), 4943 – 4951 [original: *Pure Appl. Chem.* **81**, 1131–1186 (2009)]. [Translation only of excerpts.]

S.R. Heller, A.D. McNaught: The IUPAC International Chemical Identifier (InChI), *Chem. Int.* **31** (1) 7-9 (2009).

Ida Schomburg*: Nomenklatur der Rotaxane und Pseudorotaxane, *Angew. Chem.* **121**(25), 4719-4738 (2009), translation of original: *Pure Appl. Chem.* **80**, 2041-2068 (2008)

International Chemical Identifier (InChI) Development

Several projects developing aspects of the InChI have been completed and the results incorporated into new versions of the InChI software.

Manuscripts for Recommendations or Technical Reports are being prepared for the following projects:

Terminology Relating to and Nomenclature for Macromolecular Rotaxanes and Pseudorotaxanes (IUPAC Recommendations 2011)

Revision of “IUPAC Recommendations on Macromolecular Nomenclature – Guide for Authors of Papers and Reports in Polymer Science and Technology”

Preferred IUPAC Names (PINs) for Inorganic Compounds: “Specifying the Coordination of Ligands to Central Atoms: Detailed Description of Grammar in the Kappa (κ) Convention”

Richard Hartshorn

President

IUPAC Division of Chemical Nomenclature and Structure Representation