

International Union of Pure and Applied Chemistry

Division VIII

Chemical Nomenclature and Structure Representation

Report on the Work of the Division
August 2005 to September 2006
for Bureau meeting, Madrid 2006

Annual Meeting

The division met in Prague on 6 and 7 September. Fifteen members attended (9TM, 5AM and 1NR). Dr Damhus was intending to come too but had a serious accident which prevented him travelling. On 4 and 5 September the working party on structure representation met with three other members not on the division committee.

Publications

Nomenclature of Inorganic Chemistry: IUPAC Recommendations 2005, Edited by N H Connelly, T Damhus assisted by R M Hartshorn and A T Hutton, Royal Society of Chemistry, 2005

The authors were congratulated on the new edition of the Red Book. This is a revision and update of the 1990 edition. Concern was expressed about the lack of publicity of this new edition. It was reported that at a national meeting the RSC only brought one copy which it sold almost immediately and expressed surprise anyone was interested. Another concern was when would an electronic copy be placed on the web.

Graphical representation of stereochemical configuration, *Pure Appl. Chem.* 2006, **78**(10), 1897-1970 prepared by Jonathan Brecher.

This is the first part of a two or three sets of recommendations on structure representation. It covers all aspects of how to show stereochemistry on a chemical structural diagram. This includes double bonds, chirality, conformational drawing and some of the special requirements for natural products.

Projects

IUPAC International Chemical Identifier (InChI) (project 2000-025-1-800)

A new software release, version 1.01 was released in August 2006. It is for use in Windows or Linux (i386). It now includes a validation tool and InChI to structure conversion. (success rate on average 99.7%). Work is in progress to extend its application to polymers. It was noted that the InChI could be used to search on Google. An article on it will appear in *Chemistry International* in the November issue. It was noted that at least 13 databases are using it. (see also www.inchi.info)

Preferred names for organic compounds (project 2001-043-1-800)

Work is continuing on this revision of the Blue Book. In the new book it will provide for the first time a preferred IUPAC name (PIN) but will also describe other acceptable methods of naming compounds. Although this has been to public review the revisions which that has generated require extensive work to ensure it is entirely self-consistent.

Nomenclature of rotaxanes (project 2002-007-1-800)

This project covers the nomenclature of discrete rotaxane molecules. It will be followed by a separate project on macromolecular rotaxanes. The final draft of the document following public review should be ready shortly.

Extension of IUPAC rules for stereodescriptors to coordination numbers 7-12
(project 2003-025-1-800)

After a comprehensive study of the various published methods it was concluded that there was not possible to make firm recommendations, at least for the time being. A technical report on the subject has been prepared.

Macromolecular projects (with Division IV)

These were mainly considered at the meeting of the Division in Rio de Janeiro in July 2006. Progress was reported on Source-based nomenclature for single-strand organic polymers (project 2003-042-1-800), Nomenclature and graphical representations for chemically modified polymers (project 1999-051-1-800), and Structure-based nomenclature for cyclic macromolecules (project 2001-082-1-800). In addition work is in progress on the nomenclature of macromolecular rotaxanes (project 2000-037-1-800), and Terminology and structure-based nomenclature of dendritic and hyperbranched polymers (project 2000-081-1-800).

Graphical representation standards for chemical structure diagrams (project 2003-045-1-600)

The latest draft was considered by the working party in Prague and most outstanding points dealt with. A final revision should be ready soon. The question of whether macromolecules should be included or whether a separate document should be prepared was left for further discussion. A separate document would be a revision and update of the 1994 recommendations.

Comparison of procedures for naming hydro derivatives of fused ring systems.

This was prepared as a technical report on the three methods used by IUPAC, Beilstein and Chemical Abstracts Service. As it now contains some new material derived from the preferred name project it was questioned whether it should go to public review before publication.

Other projects

No progress was reported on the Nomenclature of cyclic peptides (project 2004-024-1-800). A new project on the Nomenclature of phosphorus containing compounds of biochemical interest (project 2006-051-1-800) has been approved. This is a revision and update of the 1976 document. Two other projects are awaiting final approval. A second edition of the 1998 book *Principles of Chemical Nomenclature*, and preferred names for inorganic compounds.

Gerry Moss
Division President
29 September 2006