

## International Union of Pure and Applied Chemistry

### Division VIII

#### Chemical Nomenclature and Structure Representation

##### 1. Highlights

Since the last report there has been the publication of one of the colour books, the *Nomenclature of Inorganic Chemistry - IUPAC Recommendations 2005*, by N.G. Connelly, T. Damhus, R.M. Hartshorn and A.T. Hutton, The Royal Society of Chemistry, 2005 [ISBN 0 85404 438 8]. Often referred to as the Red Book this is a revision of the previous edition of 1990, incorporating some parts of *Nomenclature of Inorganic Chemistry II, IUPAC Recommendations 2000* (Red Book II). The organisation of the Red Book has been changed to improve clarity. An important addition to this edition is the chapter on organometallic compounds expanding a brief section previously under coordination compounds.

The IUPAC International Chemical Identifier (InChI) is making steady progress. This is a character string unique to any chemical structure, generated algorithmically by a software programme. Unlike other unique identifiers, such as the CAS registry number, it has the property that the structure can be regenerated from the InChI with a success rate of over 99%. The InChI is now being used by at least 16 major internet databases (~25 million structures) and 3 primary journals. Software developers are providing the identifier in their output. A recent proposed extension is InChI Hash, developed primarily to facilitate use of the InChI by web search engines, which break a long InChI string in unpredictable ways. It will probably be 19 characters including a check character. Although close to unique (97% probability of no collisions in 100 million structures) it cannot be converted back to the structure (see [www.iupac.org/inchi/](http://www.iupac.org/inchi/)).

Another project which has been published is "Graphical representation of stereochemical configuration (IUPAC Recommendations 2006)" *Pure Appl. Chem.* **78**(10), 1897-1970, 2006. This is the first part of the work on structure representation. The importance of clear depiction of stereochemistry is obvious. The document provides recommendations on how to unambiguously show stereochemistry and warns about other ways which may result in ambiguity.

A major project of the Division is the revision of the *Nomenclature of Organic Chemistry* (Blue Book). This has proved harder than anticipated. It is not just a revision and extension of the

existing books (*IUPAC Nomenclature of Organic Chemistry*, 1979, and *A Guide to IUPAC Nomenclature of Organic Compounds*, 1993) but also incorporates more recent recommendations published since 1993. However, for the first time, it also aims to provide, for those users who require it, a preferred IUPAC name out of the alternatives that are possible. Guidance on alternative methods of naming compounds are retained.

A number of projects are nearing completion. The "Extension of IUPAC rules for stereo descriptors to include coordination numbers 7-12" came to the conclusion a single recommendation could not be made and so it presented alternative appropriate methods for indicating the stereochemistry.

"Graphical representation standards for chemical structure diagrams" is the second part of the project on structure representation (for part 1 see above). It covers the drawing of structure excluding stereochemistry.

"Nomenclature of phosphorus-containing compounds of biochemical importance" is the revision of a 1976 document, improving presentation and adding a number of extensions to reflect recent developments. It is being supervised by the IUPAC-IUBMB Joint Commission on Biochemical Nomenclature, a sub-group of Division VIII. They provide chemical advice to the IUBMB work on enzyme nomenclature. They are also involved with "Recommendations for nomenclature and databases for biochemical thermodynamics", a revision of the 1994 document.

There are a number of projects which are joint with division IV. "Nomenclature of rotaxanes" is the first half of an old project. It deals with the discrete molecules, i.e. not including polymeric components. "Terminology and structure-based nomenclature of dendritic and hyperbranched polymers" and "Terminology and nomenclature of macromolecules with cyclic structures" are both nearly ready for publication.

An objective of the division is to extend the provision of a preferred IUPAC name from organic compounds to other compounds. The inorganic project has started work and it is hoped that a macromolecular project can be established.

The 1998 book intended for educational use *Principles of Chemical Nomenclature a Guide to IUPAC Recommendations* is to be revised to update it with changes arising from the new Red Book and draft Blue Book.

Other projects that the Division are involved with are listed in section 4.

## **2. Report on the work of the Division for the IUPAC Strategic Plan Long Range Goals**

**a.** Chemical nomenclature has implications in a wide range of disciplines. Unambiguous chemical names should be used in medicine, legal work, etc., as well as all sciences outside chemistry. Providing clear instructions for naming compounds, and which are available world wide to anyone who requires them, is an object of Division VIII.

**b.** Nomenclature is fundamental to the communication of research. The clear, unambiguous naming of compounds or drawing of their structures is a prerequisite for understanding. The Division is addressing both aspects. Representation of chemical databases on the Division committee help to ensure the widespread use of IUPAC nomenclature

**c.** Patents and other registration requirements often require preferred IUPAC names. The procedure for organic compounds has now been established, and there is a similar project for inorganic compounds. It is hoped to extend it to macromolecular compounds also.

**d.** Most nomenclature recommendations are available from the web. This has enabled world wide access even where the original publication is not readily available. The web version has then been used to translate recommendations into the local language.

**e.** The educational needs are particularly addressed by *Principles of Chemical Nomenclature a Guide to IUPAC Recommendations*, 1998. A revised edition is in preparation.

**f.** It is difficult to broaden the membership base of the division, as it is rare for a nomenclature expert in a special area to also have a broad knowledge of chemical nomenclature. However we do try to encourage the involvement of as wide a range of chemists as possible. Individual documents are of course very widely reviewed at the provisional stage.

## **3. Other substantive information.**

Since the last Council meeting the InChI project has been publicised by a number of presentations in Germany, Japan, Spain, UK and USA.

## **4. Tabular Material**

### **Publications**

*Nomenclature of Inorganic Chemistry - IUPAC Recommendations 2005*, by N.G. Connelly, T. Damhus, R.M. Hartshorn and A.T. Hutton, The Royal Society of Chemistry, 2005 [ISBN 0 85404 438 8]

Graphical representation of stereochemical configuration (IUPAC Recommendations 2006), *Pure Appl. Chem.* 78(10), 1897-1970, 2006

## **Projects**

1999-051-1-800 Nomenclature for chemically modified polymers

2000-037-1-800 Nomenclature for macromolecular rotaxanes

2001-043-1-800 Preferred names in the nomenclature of organic compounds

2001-081-1-800 Terminology and structure-based nomenclature of dendritic and hyperbranched polymers

2001-082-1-800 Terminology and nomenclature of macromolecules with cyclic structures

2002-007-1-800 Nomenclature of rotaxanes

2003-025-1-800 Extension of IUPAC rules for stereo descriptors to include coordination numbers 7-12

2003-042-1-800 Source-based nomenclature of single-strand organic polymers

2003-045-3-800 Graphical representation standards for chemical structure diagrams

2004-024-1-800 Nomenclature of cyclic peptides

2004-039-1-800 IUPAC International Chemical Identifier (InChI): promotion and extension

2006-019-1-800 Nomenclature of phosphorus-containing compounds of biochemical importance

2006-029-1-800 Revision of "*Principles of Chemical Nomenclature*"

2006-038-1-800 Preferred IUPAC Names (PINs) for Inorganic Compounds

2006-023-3-100 Recommendations for nomenclature and databases for biochemical thermodynamics