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Last update: 12 August 2009

Project: Graphical representation standards for chemical structure diagrams

Objective

To extend IUPAC's leadership in the development of standard nomenclature and terminology in chemistry into the domain of chemical structure diagrams.

To provide a single, comprehensive set of guidelines for creating chemical structure diagrams in printed and in electronic media.

To enable IUPAC to serve as the principal, authoritative source for chemical structure representations.

Description

Although some existing IUPAC nomenclature recommendations already discuss some aspects of chemical structure diagrams, they do so only tangentially. Even if they were to be collected in one location, these existing recommendations on chemical structure diagrams are incomplete, and do not discuss many basic issues. As a result, many organizations have formulated their own guidelines for creating chemical structure diagrams; however, none of those guidelines is comprehensive. Provision of a single, comprehensive set of guidelines for creating chemical structure diagrams would be a significant benefit to the chemistry community.

The project has begun informally with a "scoping exercise" in which some 20 members of the chemistry community were invited to discuss those aspects of creating chemical structure diagrams which are amenable to standardization through IUPAC recommendations. Some draft recommendations were created during the course of that scoping exercise, and these will serve as a useful starting point (See www.angelfire.com/sc3/iupacstructures/). The participants in the scoping exercise also identified several areas that are likely to be contentious or otherwise were incompletely specified; those areas will receive specific attention during the course of the project. We are excluding polymer representations for now but if time permits we will address polymers and add one or more names of polymer nomenclature experts to the task group.

With the ever-increasing importance of electronic publication, this project will consider issues related to the production of chemical structure diagrams both in printed and in electronic media. Where possible, every effort will be made to ensure identical recommendations in all media. The recommendations for the production of chemical structure diagrams will aid in the correct recognition of structural information by the [IUPAC/NIST Chemical Identifier algorithm](#).

In some cases, the current state of chemistry software may preclude the use of the most-preferred styles for chemical structure diagrams. When necessary, this project will also provide practical advice for the production of electronic chemical structure diagrams according to the current state of the art of chemistry software. It is likely that this project will also produce a set of recommendations for enhancements that chemistry software developers may undertake to improve that state of the art.

Progress

This project was presented at a [poster session](#) at the IUPAC Congress/GA July 2005

Number: 2003-045-3-800

Start: 01 March 2004

End: 18 February 2008

Project of

[Chemical Nomenclature and Structure Representation Division](#)

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The first IUPAC Recommendations on this topic, titled 'Graphical representation of stereochemical configuration' has been published in [Pure Appl. Chem. 78\(10\), 1897-1970, 2006](#).

A second manuscript titled 'Graphical Representation Standards for Chemical Structure Diagrams' is being prepared for publication in Pure Appl. Chem. A draft is submitted to public review comments until 30 June 2007.
> see provisional recommendations [[../reports/provisional/abstract07/brecher_300607.html](#)]

Feb 2008 - *Project completed* - IUPAC Recommendations published in [Pure Appl. Chem. 80\(2\), 277-410, 2008](#).

<project announcement published in [Chem. Int. Jul-Aug 2004 issue](#)>