Basic Terminology of Crystal Engineering

Crystal engineering is the design and synthesis of functional crystalline structures, based on a bottom-up approach from smaller building blocks. Crystal engineering is a fascinating new subject that has expanded rapidly in the last 20 years. It is also attracting the interest of the chemical and pharmaceutical industry. It overlaps with supramolecular chemistry, X-ray crystallography, materials science, and solid-state chemistry, but is a distinct discipline in itself. The subject goes beyond the traditional divisions of organic, inorganic, and physical chemistry; this makes for an eclectic blend of ideas, techniques, and strategies.

The diversity in focus and scientific basis of the researchers in the field has led to numerous terminology practices that are not consistent among research groups, causing confusion and unnecessary conflicts.

The purpose and scope of this project is to provide a basic glossary of terms for this rapidly evolving, highly interdisciplinary field, to identify and debate open questions, and to point out new directions.

The objectives of this project are: to produce guidelines for terminology (glossary of terms) in the area of crystal engineering; to ensure that these guidelines are accepted by a large group of leading researchers in the field; and to have these guidelines implemented or referred to in the instructions to authors of leading crystal engineering journals.

In May 2014, the Task Group secured a grant from ICSU and proceeded with a kickoff workshop held concurrently with the 1st International Symposium on Halogen Bonding (ISXB-1) in Porto Cesareo (Lecce, Italy), 18-22 June 2014 (see http://www.isxb-1.eu/symposium-program/satellite-event.html). The project is being advertised in major meetings relevant to related fields, including the recent 23rd Congress and General Assembly of the International Union of Crystallography (IUCr) held in Montreal, Canada, 5-12 August 2014.

Next year, 30-31 August 2015, an international workshop open to the public will be organized for consideration of public comments, presentation, and dissemination of results; the workshop will be a satellite event, part of the 29th European Crystallography Meeting organized in Croatia.

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www.iupac.org/project/2012-044-1-100

Implementation of InChI for chemically modified large biomolecules

The IUPAC International Chemical Identifier (InChI) algorithm is now well established as a powerful means of denoting the basic chemical structure of a well-defined, small (<1024 atoms) organic molecule as a unique machine-readable character string, suitable for electronic data storage, searching, and exchange. The IUPAC Division VIII InChI Subcommittee is now starting work on a complete overhaul of the InChI algorithm, i.e. the beginning of plans for a second version of InChI. A crucial part of this work is intended to address the known shortcomings of the current InChI algorithm pertaining to the handling (or lack thereof) of various types of biological substances. Chemically modified sequences are becoming very important in life science research both as tools and as products. Chemically modified biologics range from siRNA sequences, established therapeutics such as Levimir and Byetta for diabetes, to the growing area of antibody drug conjugates (ADCs). There is currently no standard approach for the naming of chemically modified biologics; this constitutes a tremendous opportunity for InChI to become established as the naming technology.

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www.iupac.org/project/2013-010-1-800

Toxicology in the Classroom II

This new project is based on a recently completed IUPAC project 2004-045-1-700 "Training of School Children on Pesticides and Health" that was designed to raise awareness among young children about the potential adverse effects of chemicals and, in the process, help reduce the careless use of pesticides. Toxicology in the classroom (Toxiclaro for short) is a multimedia resource that will help teachers educate their students about pesticides and health. Toxiclaro is a virtual toolbox, offering training materials, a curriculum, and resources such as games, experiments, and a virtual house to explore—all of which provide for a basic understanding of toxicology and awareness of the need for protective and precautionary measures.

Task group members prepared an experimental design for teaching the dose response principle in the classroom. This experiment makes use of the suppression of seed growth by copper sulfate. A test run was