The Project Place

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See also www.iupac.org/projects

NMR Chemical Shifts: Updated Conventions

The recent IUPAC document on conventions for chemical shifts (*Pure and Applied Chemistry* **73**, 2001, 1795), which has been well received by the nuclear magnetic resonance (NMR) community, left a number of outstanding issues for later debate. These include (i) temperature variation of the signals for the standards, (ii) the use of magic-angle spinning for both solutions and solids, (iii) solvent effects, (iv) susceptibility measurements/corrections, and (v) conventions for shielding tensors. These matters will now be taken up by a Task Group including R. K. Harris (chairman), E. D. Becker, S. M. Cabral de Menezes, P. Granger, and K. W. Zilm. An evening "open forum" has been arranged during the 16th International NMR Meeting on NMR Spectroscopy at the University of Cambridge, 29 June to 3 July 2003, to discuss the relevant questions.

Anyone with views or information about these issues should contact either <r.k.harris@durham.ac.uk> or <tbecker@nih.gov>.

www.iupac.org/projects/2003/2003-006-1-100.html

Terminology for Radical Polymerizations with Minimal Termination

About 10 years ago it was discovered that the addition of certain compounds—e.g., nitroxides or complexes of Cu(I)—had a profound effect on the course of a radical polymerization. The radicals formed are then able to persist for long periods, consequently the molecular weight of the polymer produced increases with conversion, resulting in low polydispersity. In their enthusiasm for novel reactions of this kind, the authors of papers describing their results developed individual types of nomenclature without any coordination.

The frenzy of activity on the part of individuals outside IUPAC to attempt to define terms, or to call for regulated terminology, demonstrates the urgent need for an appropriate IUPAC body to quickly provide an internationally agreed set of terms in this field of the so-called "living" and/or "controlled" radical polymerization. The IUPAC Subcommittee on Macromolecular Terminology wishes to resolve these issues with a minimum of delay.

For more information contact the Task Group Chairman Aubrey D. Jenkins at <adjjj@jjadj.u-net.com>.

www.iupac.org/projects/2002/2002-006-2-400.html

Toward a Core Organic Chemistry Curriculum for Latin American Universities

The Committee on Chemistry Education (CCE) and the Organic and Biomolecular Chemistry Division have jointly endorsed a project with the following objectives:

- to propose general recommendations for up-to-date university curricula in organic chemistry without interfering with instructors' freedom
- to contribute to the public understanding of chemistry by introducing fundamental concepts that demonstrate how organic chemistry is important to most aspects of common life
- to facilitate communication, transferability of courses, and exchange of students, as well as insertion of graduates into transnational industries

CCE proposes that this be a pilot project focused on Latin America. The goal is not to unify curricula worldwide, but instead to concentrate on a region where there is a demonstrable interest. If successful, the project might be extended to other developing countries and/or regions.

The Task Group proposes to develop recommendations for curricula in organic chemistry, including a set of required and recommended topics to be covered at each educational level in a university. One goal is to ensure that students reach an acceptable level of knowledge by the end of their course of studies, without undue gaps. There is no intention of imposing a uniform curriculum; the aim is to define what new material should be introduced and what can be deleted or reduced. A similar project was recently undertaken in Europe, in which more than 200 universities have been developing the European Chemistry Thematic Network <www.cpe.fr/ectn>.

The initial Task Group, which included members from Argentina, Chile, Brazil, Mexico, and Europe, have exchanged information and classified topics as essential, desirable, or non-essential. Since the project began in the summer of 2002, the Task Group has made good progress, in part because it has grown to include new members. An informal meeting was first held in August 2002 in conjunction with the 16th IUPAC Conference on Physical Organic Chemistry (ICPOC16), San Diego, California, USA. The participation of other conference attendees resulted in very stimulating discussions and suggestions and valuable input from a number of organic chemists. The project was later presented as a

plenary lecture at the XXV Latin-American Congress of Chemistry in September 2002, where it resulted in a full and wide-ranging discussion.

The Task Group has now identified a number of key issues, including the range of backgrounds of students entering the course, the stimulation of interest, emphasis on social responsibility, the introduction of material in a regional context, the provision of courses for non-majors and students of the humanities, transferability between courses, and the dissemination of the final recommendations and conclusions. Future discussions will include the identification of essential topics and the number and type of courses. These issues will be explored over the following months and reported on later.

For more information, contact the Task Group Chairman Norma S. Nudelman at <nudelman@qo.fcen.uba.ar>.

www.iupac.org/projects/2002/2002-010-1-050.html

Rules for Stating When a Limiting Value is Exceeded

This is a brief summary of an IUPAC activity carried out under the Chemistry and Human Health Division. The former Commission of Toxicology (COMTOX) has established a set of rules for stating whether or not a measurement result is in conformity with given specifications.

Conformity testing is a systematic examination of the extent to which a measurement result indicates that the value of the measurand (e.g., the concentration of a substance in a matrix) conforms or not with a given limiting value. This procedure has some very well-known and practical applications, such as detecting doping in sports, alcohol levels in drivers' blood, levels of toxic metals in workers' blood, the proportion of gold in alloys, and the amount of pesticides in drinking water. The objective of the rules for stating when a limiting value is exceeded is to provide assurance of conformity, either in the form of a supplier's declaration, or of a third-party certification. A specification is usually formulated as a single limiting value or upper and lower limiting values. The assurance may be in the form of a supplier's declaration or of a third-party certification.

When conformity testing involves measurement or sampling uncertainty, it is common practice to use elements from the theory of statistical hypothesis testing to provide a formal procedure. If you know the measurement procedure and if you can determine a level of uncertainty for that measurement, you can also estimate and minimize the risk of making errors in claims of conformity or non-conformity to the particular specifications. The description of the rules was published by Christensen et al. (Christensen JM, Holst E, Olsen E, Wilrich PT. Rules for stating when a limiting value is exceeded. *Accred. Qual. Assur.* **7**, 28-35 [2002]).

Test for Conformity Versus Test for Non-Conformity

Different tests exist for conformity and non-conformity. Which one you use depends on the consequences of a wrong statement. An example of a test for conformity is an investigation of the amount of poesticide in a drinking water supply system that serves several hundred thousand people. A declaration that the concentration of the pesticide is below the limiting value—i.e., the point at which that water supply is deemed unsafe—should be made with great confidence. On the other hand, a test for non-conformity might involve measuring the alcohol concentration in a driver's blood. A declaration that the blood-alcohol concentration in a particular driver exceeds the limiting value—i.e., that person is driving while drunk—should also be made with great confidence.

A test for conformity must always result in only one of the following statements:

- Statement A: The measurement results have demonstrated beyond any reasonable doubt that the value of the measurand is in conformity with the requirement.
- Statement B: The measurement results have demonstrated beyond any reasonable doubt that the value of the measurand is not in conformity with the requirement.
- Statement C: The measurement results have not been able to demonstrate beyond any reasonable doubt whether the value of the measurand is or is not in conformity with the requirements.

The rules for testing conformity are as follows:

Rule 1: For a one-stage testing procedure, conformity with the requirements is declared, if and only if, the uncertainty interval for the value of the measurand is inside the region of conformity.

Rule 2: For a two-stage testing procedure, conformity with the requirements is declared, if and only if, the uncertainty interval for the value of the measurand is inside the region of conformity either after the first stage or after the second stage. The second stage of the test is performed if, and only if,