

Public Understanding of Science: Identifying IUPAC's Niche

Enhancing the public understanding of science means different things to different stakeholders, and has different meaning in the diverse global contexts represented by the IUPAC community. Yet, enhancing the public understanding of chemistry is a key element of IUPAC's mission. Because a large number of other organizations are already active in the field, determining the particular role that IUPAC can and should play, without reinventing the wheel, requires careful analysis. The Committee on Chemistry Education (CCE) approved a project that aims to help identify appropriate involvement for IUPAC in this area, as well as to give direction to the CCE, which is charged with fostering public understanding through its work to improve chemistry education.

The project will have four stages:

1. A workshop for the task group members to prepare a preliminary report, with recommendations, on effective public understanding of science initiatives based upon a review of the literature. The workshop will be held over three days in Edmonton, Canada, in May 2005.
2. A special workshop within the Beijing IUPAC General Assembly in August 2005 to consider the report from (1) above and to produce a draft report to the IUPAC Bureau on the role for IUPAC in promoting public understanding of science. Participants would be the Task Group; CCE—including the Associate Members representing the scientific divisions of IUPAC; representative(s) of the Committee on Chemistry and Industry (COCI); CHEMRAWN; and others that the IUPAC Executive Committee may nominate. The report will identify what further work, if any, needs to be undertaken to develop an IUPAC consensus on the role and strategy of IUPAC in the public understanding of

science. Following the creation of that draft report, there would be consultation within IUPAC on those findings, with feedback to the Task Group.

3. A symposium within, and other contributions to, the 19th ICCE on Chemistry and Chemical Education for Humanity in Korea in August 2006. The workshops in (1) & (2) will inform the development of the program which will stimulate further advice on IUPAC's role and strategy.
4. Task group members will attend the 19th ICCE and produce a final report based upon the feedback from consultations. The report will be to the IUPAC Bureau enabling it to determine its role and strategy on public understanding of science and to engage with other scientific unions, ICSU, and other stakeholders to agree on overarching strategy and associated activities.

All task group members are members of the CCE subcommittee on the Public Understanding of Chemistry, and include Peter Mahaffy, Bob Bucat, Tony Ashmore, and Choon Do. The group welcomes your comments and suggestions on "best practices" and appropriate roles for IUPAC in building public understanding of chemistry. Contact Peter Mahaffy <peter.mahaffy@kingsu.ca> with your suggestions.



www.iupac.org/projects/2004/2004-047-1-050.html

Uncertainty Estimation and Figures of Merit for Multivariate Calibration

With the ever-increasing sophistication of analytical instruments, multivariate calibration methods are continually evolving, each with its own underlying assumptions and statistical properties. The main purpose of these methods is to produce valid predictions from highly unselective data (e.g., the quantification from near-infrared spectra). A wide variety of multivariate methods have been developed, broadly classified in terms of the tensorial order of the instrumental data. Important conceptual differences exist between first-order methods employing vector data, and second-order methods using matrix data, particularly since the latter make possible the quantification in the presence of unknown interferents. This is also reflected in the approaches followed for the estimation of figures of merit.

While univariate calibration leads to relatively sim-



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ple models, and the associated uncertainty estimation and figures of merit are thoroughly covered in several official documents, multivariate calibration does not enjoy a similar status in this regard. Uncertainty estimation and figures of merit for multivariate calibration methods have become subjects of active research, especially in the field of chemometrics.

This work is intended as an introduction to multivariate calibration from a chemometrics perspective and as a review of the various proposals to generalizing the well-established univariate methodology to the multivariate domain.

Uncertainty and figures of merit are subjects of interest to IUPAC's Analytical Chemistry Division, as established within the general aims of the Division, and also in the terms of reference of its Interdivisional Working Party on Harmonization of Quality Assurance.

For more information and comments contact the Task Group Chairman Alejandro C. Olivieri <aolivier@fbioyf.unr.edu.ar>.

 www.iupac.org/projects/2004/2004-041-1-500.html

A Joint OPCW–IUPAC Project on Education and Outreach Regarding Chemical Weapons

In the IUPAC report on chemical weapons (*Pure Appl. Chem.* **74**(12), 2323–2352, 2002), stress was laid on the importance of spreading knowledge of the Convention on Chemical Weapons and educating chemists and the public on the ethical aspects of these

terrible applications of our science. The Committee on Chemistry Education (CCE) is charged with overseeing educational aspects of IUPAC's activities, and the matter came before the committee at its meetings. The committee was uncertain about how to proceed, for there is a fine line between educating in favor of prohibition and educating, accidentally, for propagation. At its meeting in Istanbul in August 2004, the CCE established a working party (led by



Natalia Tarasova) to explore the question of how to proceed.

To take the matter forward, IUPAC President Leiv Sydnes and Task Group Chairman Peter Atkins established contact with the Organization for the Prohibition of Chemical Weapons (OPCW), based in The Hague, and attended the States Signatories session in January 2005. From that meeting, and a particularly fruitful meeting with Ralf Trapp (OPCW), we found a way forward. A meeting now planned for next July will explore the feasibility of a conference to discover if there are ways ahead in addressing problems of insinuating ethical aspects into already overburdened chemical curricula. Readers who have strong views are encouraged to send them to Atkins, who will try to compile a discussion document for the coming meeting.

For more information and comments contact the Task Group Chairman Peter Atkins <peter.atkins@lincoln.oxford.ac.uk>.

 www.iupac.org/projects/2004/2004-048-1-020.html

Categorizing Hydrogen Bonding and Other Intermolecular Interactions

This project aims to 1) take a comprehensive look at intermolecular interactions and classify them and 2) create a modern definition of the hydrogen bond, taking into account all current experimental and theoretical information, and including hydrogen bonded systems both in gaseous and condensed phases, as well as in chemical and biological systems.

Hydrogen bonding has fascinated chemists and biologists for several decades now and is central to chemistry and biology. The original definition of hydrogen bonding invoked two electronegative atoms (X and Y) interacting through a hydrogen atom as in X–H...Y. Initially X and Y were found to be mostly N, O and F which led to the mentioning of these atoms as part of the definition of hydrogen bonds in various sources (including the IUPAC Gold Book). Hydrogen bonding was inferred by the difference in physical properties between otherwise chemically similar systems such as are found between H₂O and H₂S. However, now it is well known that both H₂O and H₂S form a hydrogen bonded (H₂X)₂ dimer in the gas phase. Spectroscopic red shift in XH stretching frequency was among the first experimental evidence