The Project Place

Information about new, current, and complete IUPAC projects and related initiatives.
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Solubility and Thermodynamic Properties Related to Environmental Issues

Solubility is a basic phenomenon that determines the extent of most pollution problems, both environmental and industrial. However, no book is currently available on the importance of solubility and thermodynamic properties to environmental issues.

The objective of this project is to publish a 25-chapter book on recent developments in solubility and in thermodynamics that have a bearing on environmental issues. This, we the project leaders believe, could lead to new ways of thinking about and solving environmental problems. In true IUPAC style, the authors of this book have been drawn from 17 countries.

The chapters focus on such areas as predicting and modeling of environmental pollutants from basic thermodynamics considerations; designing remediation and cleaner industrial processes; predicting and measuring the uptake of pollutants and new industrial chemicals in humans and in animals; and environmental issues related to health science, mining, pesticides, soil chemistry, supercritical and phase equilibria separation processes, gasoline additives, ionic liquids in industry, corrosion control, surfactants, green synthesis, surface adsorption, and biodegradeable plastic films.

The book is scheduled to be published in 2007. Another book on Developments and Applications in Solubility is the subject of a separate project and is scheduled to be published later in 2006.

For more information and comments, contact the Task Group Chairman Trevor Letcher <trevor@letcher.eclipse.co.uk>.

www.iupac.org/projects/2005/2005-048-2-100.html

Terminology for Self-Assembly and Aggregation of Polymers

With nanoscience and nanotechnology enabling many of the key developments in modern functional materials, aggregation and self-assembly in polymers is of growing importance. The physical and chemical properties of aggregated polymers and polymer molecules that spontaneously assemble into ordered structures are more often determined by these macroscopic structures than by the individual polymer molecules from which they are built. Many of the terms used to describe the different aggregated structures and self-assemblies, their methods of formation, their characterization, and any related terminology might be totally unfamiliar to scientists whose background is not in this discipline.

This project, therefore, will develop a list of terms and definitions for chemists and materials scientists within academia and industry. The definitions will be harmonized for acceptance by the chemistry, polymer, and materials communities. To assist in achieving this assent, members of the learned societies of different countries will be consulted to ensure that the definitions are accepted worldwide.

For more information, contact Task Group Chairmen Christopher Ober <cober@ccmr.cornell.edu> or Richard Jones <dick@rgjones.freeserve.co.uk>.

www.iupac.org/projects/2005/2005-043-2-400.html

Nomenclature of Phosphorus-Containing Compounds of Biochemical Importance

The objective of this project is to update and clarify recommendations for naming phosphorus-containing compounds. Many of these compounds are extremely important in biochemistry and hence in nearly all branches of biology and medicine. Most biochemically important compounds are esters and/or anhydrides of various phosphorus-containing acids with complex organic alcohols and organic acids.

Existing recommendations, available at <www.chem.qmul.ac.uk/iupac/misc/phospho.html>, have not been revised since 1976; since that time, much more has become known about many classes of phosphorus-containing compounds (e.g., inositol phosphates). The Chemical Nomenclature and Structure Representation Division (VIII) and the IUBMB-IUPAC Joint Commission on Biochemical Nomenclature are supporting this project in recognition of the need to redraft the recommendations more clearly, define the symbols used, and use as examples compounds that feature widely in biochemistry.

For more information, contact Task Group Chairman Hal Dixon <h.b.f.dixon@bioc.cam.ac.uk>.

www.iupac.org/projects/2006/2006-019-1-800.html

Determination of Selenomethionine in Selenized Yeast Supplements

Production and consumption of Se supplements have increased dramatically in recent years as yeast-based supplements have emerged as an acknowledged means of alleviating selenium nutrient deficiencies for both animals and humans. However, it is evident from earlier studies that these supplements are often inconsistent in their makeup relative to label indications.

Significant efforts have been made in the development of analytical methods for the speciation of Se in yeast in recent years [selenomethionine (SeMet) is the dominant Se species in yeast-based Se supplements]. Extraction procedures used are of paramount importance for the accurate determination of SeMet in yeast or other solid samples, and numerous ones have been developed. However, there remains a lack of consensus regarding whether there are forms of selenium other than SeMet in yeast. Consequently, the four major industrial companies producing selenized yeast boast their SeMet content as a proof of the quality of their yeast without a consensus existing on the methodology used and the validity of the measurements supplied.

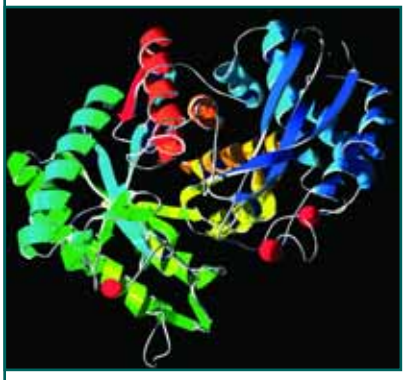


Illustration depicts a 3D model of the yeast enolase protein, showing three areas of selenomethionine incorporation (red dots). *Image reproduced by permission of Zoltan Mester and The Royal Society of Chemistry from The Analyst, 2005, 130, (1), cover page © Crown Copyright of Canada.*

The purpose of this project is to examine existing methodologies published in peer-reviewed journals and issue recommendations on the determination of this extremely important nutritional supplement. The task group is composed of five scientists with considerable experience in the field, and the work will be carried out in close collaboration with the potential stakeholders.

For more information, contact Task Group Chairman Zoltan Mester <zoltan.mester@nrc.ca>, Canadian national representative to the IUPAC Analytical Chemistry Division, Institute for National Measurement Standards National Research Council, Ottawa, ON, K1A 0R6, Canada.

www.iupac.org/projects/2005/2005-041-2-500.html

Selection and Use of Proficiency Testing Schemes for Limited Number of Participants (Chemical Analytical Laboratories)

The IUPAC Interdivisional Working Party on Harmonization of Quality Assurance has recently revised the international harmonized protocol for the proficiency testing (PT) of (chemical) analytical laboratories. The IUPAC Technical Report was published in *PAC* 78(1), 145–196, 2006.

However, PT schemes described in the protocol were developed mostly for a relatively large number of laboratories-participants (more than 20 to 30). These laboratories form a representative statistical sample from the corresponding theoretical population of an infinite number of participants. Even if analytical results of the laboratories–participants are distributed arbitrarily, the sample mean distribution is close to the normal one. Therefore, the assigned/certified value of the PT test material can be calculated from the PT participant results as a consensus value [i.e., as the mean (or the median) of the results]. The performance of these participants is assessed based on the difference between their results and the assigned value.

The problem is that even for 30 participants, their (statistical) sample mean and standard deviation differ significantly from the corresponding population characteristics. For fewer than 30 participants, the difference between the sample and the population values is increasing with decreasing the number of participants, especially dramatically when it is less than 20.

Moreover, if the size of the population of laboratories is not infinite, and the size of the statistical sample is more than 5 to 10 percent of the population size, the ratio between the sample and the population sizes should be taken into account. In addition, not only are the sample mean or median of laboratory results biased in general from assigned/certified value (to be traceable to SI units), the population mean and median can be biased as well.

Thus, selection and use of a PT scheme for a limited number of participants (less than 20 to 30) are not routine tasks. Such schemes are quite often required for analysis of materials and/or for environmental analysis specific for a local region, for an industry under development, for analysis of unstable analytes, for a local laboratory accreditation body to control the performance of numerous unaccredited laboratories,

and so forth. Therefore, the aim of the project is to develop guidelines that could be helpful for PT providers and accreditation bodies in solving this task.

For more information, contact Task Group Chairman Ales Fajgelj <A.Fajgelj@iaea.org>.

www.iupac.org/projects/2005/2005-019-2-500.html

Young Ambassadors for Chemistry in Korea

As Korea celebrates 2006 as the Year of Chemistry, the Korean Chemical Society hosted a Young Ambassadors for Chemistry (YAC) workshop in Gwangju in the southern part of South Korea. The event took place from 20–24 February 2006 at the Chonnam National University in Gwangju.

YACs is a project of the Committee on Chemistry Education (CCE) and the Science Across the World program; its aim is to increase the public's understanding of chemistry using young people to mediate between chemistry and the general public. The students (age 10–18) perform chemistry-related activities at public locations and explain what they are doing to the passers-by, who are usually unable to keep away from the interesting hubbub they witness taking place among the group of children. The event in Gwangju was the fourth YAC event, following on the heels of others held over the past two years in Taipei, Taiwan; Buenos Aires, Argentina; and Krasnoyarsk, Russia.

The line of cosmetics developed by the students.

Train the Trainers

Prof. Choon Do, the Korean representative to CCE, organized and hosted the event and translated all event materials into Korean (the materials are downloadable from the Science Across the World Website <www.scienceacross.org> for all Korean teachers).

The event included a four-day training program for middle-school science teachers, high-school chemistry teachers, and English teachers from around the region, as well as guests from Taiwan and Japan. The English teachers played an invaluable role at the event, stepping in to help interpret when we couldn't make ourselves understood and helping create a truly collaborative, multilingual experience.

Production of the cosmetics.

On Monday, teachers carried out activities from the Science Across the World topics "Chemistry in our Lives" and "Talking about Genetics around the World"—including counting the number of taste buds on each others' tongues and surveying variation in their own group in the classroom.

On Tuesday, we carried out a "Post-It" debate on the issue of genetic science. At the same time, the teachers discussed the chemical "products" that students would produce and the advertisements for them they would prepare.

Colleagues were invited to subscribe to the Science Across the World program and join more than 5 000 teachers in some 120 countries in exchanging cultural

Students perform television commercials for the cosmetics.

and scientific information. The teachers coped extremely well with the English-language website; although the site is available in many languages, Korean is not yet one of them.

On Wednesday, teachers built a model of DNA from local sweets, successfully managing the challenge of melting marshmallows, and produced their own cosmetics. Thursday featured planning and preparation for Friday, when the teachers would help their learners perform these same chemistry-related activities in a public place.

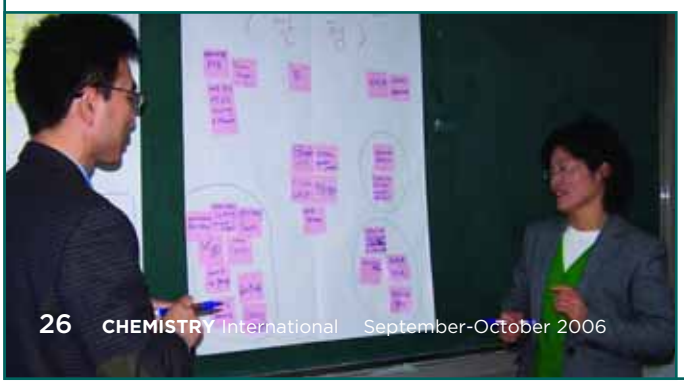
The day ended with an evaluation of the week and a discussion of the future. The participants reported that they liked the hands-on activities that helped to enhance motivation and relate chemistry to everyday life. They appreciated the chance to improve their presentation skills, particularly in English. They also expressed an interest in organizing additional YAC events and in having the chance to learn more and further their international collaboration. In particular, they expressed an interest in topics related to drinking water, conservation and recycling, renewable energy, diet and food, keeping healthy, fieldwork, dyes and coloring, and science games.

YAC Day

The YAC Public Understanding Event got started at the Gwangju bus terminal around 10:00 a.m. The teachers and about 70 students gathered to conduct science activities aimed at enhancing public interest in chemistry.

The candy DNA the students built grew longer and longer, advertising campaigns were prepared, groups delivered their product presentations, the final length of DNA was put together, and prizes and gifts were handed out to the participants.

Moderators of the "Post-It" Debate.



All told, 3 600 visitors viewed the event, the press covered it (see <www.ikbc.net>), the teachers and students worked together confidently, the weather was glorious, and everybody had a great time with chemistry—the whole point of the event.

All of the teachers who participated in the event worked hard and were very patient—particularly with our interpretation challenges. Prof. Choon Do, who was the host and organizer, discussed the event at the 19th ICCE conference held in Seoul in August 2006.

The following partners also helped make this event a success:

- Korean Chemical Society <www.kcsnet.or.kr>
- National Chonnam Normal University, Prof. Wang Keun Lee
- National Science Council
- British Council, Seoul <www.britishcouncil.org/korea.htm>, and Director Gavin Anderson
- GlaxoSmithKline <www.gsk.com>, who is the main sponsor of the Science Across the World program and who sent goody bags for all participating teachers and students

In addition, Cognis Korea <www.ko.cognis.com/korea/kocognis.html> donated the main ingredient used in preparing the shampoo and BioRad <www.biorad.com>, Life Science Education, donated the "Genes-in-a-Bottle Kit" that enabled students to extract their own DNA.

This report was prepared by Lida Schoen, science education consultant, and Keith Kelly, language education consultant. Schoen is a titular member of IUPAC CCE, team member of Science Across the World, and task group chairman for the initial YAC project. Kelly is FACTWorld coordinator <www.factworld.info> and NILE associate trainer <www.nile-elt.com>.

For more information, contact Lida Schoen <amschoen@xs4all.nl>.

www.iupac.org/projects/2003/2003-055-1-050.html

Adjustment, Estimation, and Uses of Equilibrium Reaction Constants in Aqueous Solution

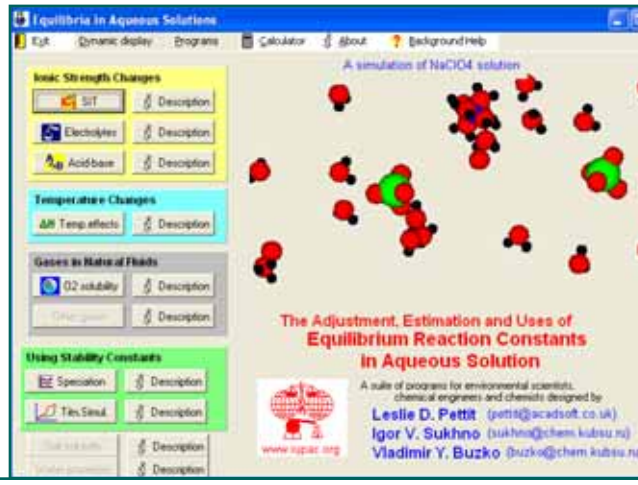
IUPAC project #2000-003-1-500 has produced a suite of programs to study quantitatively the influence of ionic strength changes on equilibrium constants, with particular emphasis on using specific interaction theory (SIT). This new project is intended to extend this previous work in the following ways:

- apply Pitzer parameters in a more general way to equilibria of environmental and industrial importance, with particular importance given to seawater and mixed fluids
- extend and improve a database of published SIT- and Pitzer-related parameters that can be accessed by all relevant programs in the suite and may be edited by the user
- extend the package to cover other environmentally important gases such as air, H_2, N_2, rare gases, N_2O, CH_4, and other paraffins (currently the package allows calculations on the effects of dissolved O_2)
- explore and test ways of displaying graphically the relationship between ionic strength and temperature with activity coefficients lg K^0 and lg K
- explore and test ways of displaying graphically the effects of errors on the relationships studied above
- calculate and demonstrate graphically the effect of errors on species distribution curves
- provide the outline of a database of reliable literature values of the dependence of stability constants on temperature

The current version of the suite of programs (Aq_solutions.zip, about 7 MB) is available from project #2000-003-1-500.

For more information, contact Task Group Chairman Igor Sukhno <sukhno@chem.kubsu.ru>.

www.iupac.org/projects/2006/2006-010-1-500.html



Design of Polymer Education Material for French-Speaking Countries

The need for a standard in polymer education has been recognized by French-speaking academics in both emerging and developed countries. The aim of this project is to set up a basic course at the undergraduate level for French-speaking countries that takes into account their local contexts. This course will be illustrated with attractive materials (e.g., a database, teaching documents, videos) provided by partners of the project and will be made available free of charge to the education community.

Task group participants (from left): P. Degee (Belgium), D. Jhurry (Mauritius), H. Kaddami (Morocco), A. Soldera (Canada), M. Popa (Romania), and G. Froyer (France).

The first meeting of the project was held at the Institut des Matériaux Jean Rouxel in Nantes, France, on 9–10 June 2006, under the sponsorship of the Université de Nantes. At this workshop, participants further improved the standard program that has been proposed via e-mail exchanges during the previous year. Attendees worked on existing available materials such as CDs and videos, rating their quality, appearance, and scientific consistency. This exercise gave them a better picture of how the polymer course should be mounted and how to make it as attractive as possible for the undergraduate students.

The group decided to share the task of mounting the polymer course among five subgroups, each one having responsibility for designing a specific part of the agreed-upon standard course. A follow-up meeting is planned for mid-2007 to validate the work done by the different subgroups.

For more information, contact Task Group Chairman Gerard Froyer <gerard.froyer@cnrs-imn.fr>.

www.iupac.org/projects/2004/2004-037-1-400.html