

## Chemistry's Contributions to Humanity—A Feasibility Study

The objective of this new project, titled "Chemistry's Contributions to Humanity—A Feasibility Study," is to evaluate the feasibility of developing a Web site that chronicles historical innovations in chemistry that have contributed to the improvement of human life. This site could serve as a source of information and education that would enhance interest in and public appreciation of the enormous contributions that chemistry has made over the past 150 years to the betterment of mankind.

Much work has been done in the past and continues today to educate the public about chemistry and its value to society and to bring balanced understanding about the benefits and risks of chemicals. Consistent with its goals, a possible role for IUPAC is to collate and integrate this array of information so that it is a more valuable resource for students, teachers, policy-makers, members of the chemical enterprise, columnists, and the general public. IUPAC can be at the helm of an international effort which will produce an authoritative source of information on the ways in which chemistry and the industries based on the chemical sciences contribute to a better life.

A Web site that portrays major innovations in chemical science over the past century and a half in an interesting and informative format could help in this task. The site would contain an encyclopedia of major chemical accomplishments that have contributed to the betterment of the human condition. It could include a detailed information base of chemical innovations and developments and permit viewing this information through a variety of queries. In short, the Web site would provide a flexible, "living" macro- and micropedia that could grow and develop in sophistication as needs developed and changed.

This is a very ambitious project—one that will take years to complete and require substantial resources. The immediate focus of the current proposal is a comprehensive analysis of the feasibility and potential value of the overall project.

The task group is particularly interested in any published or public Web site information (in English) on the theme of the "value of chemistry to society." Such information will be useful both to include in a bibliography of what is available today and to assess whether IUPAC can add value in providing a comprehensive Web site on this subject. Any person who has information to contribute to the project is urged to

contact the task group chairman or any task group members (see project web page below for details).

For more information, contact the Task Group Chairman Ed Przybylowicz <[eprzy@rochester.rr.com](mailto:eprzy@rochester.rr.com)>.



[www.iupac.org/projects/2003/2003-022-1-020.html](http://www.iupac.org/projects/2003/2003-022-1-020.html)

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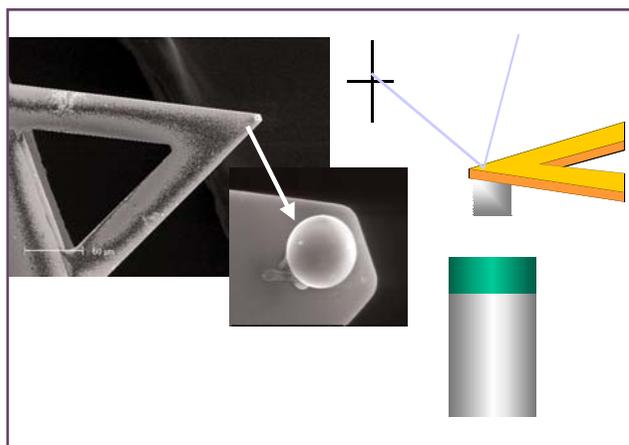
## The Use of AFM in Direct Surface Force Measurements

The atomic force microscope (AFM), more correctly described as a scanning probe microscope, can trace its origins to the scanning tunneling microscope originally invented by Binnig and Rohrer. The AFM is aimed at providing high-resolution topographical analysis for both conducting and non-conducting surfaces. The basic imaging principle is rather simple. In a common configuration, a sample attached to a piezoelectric positioner is rastered beneath a sharp tip attached to a sensitive cantilever spring. The alternative arrangement of a moving tip and a fixed sample is also possible. Undulations in the surface of the sample lead to a deflection of the spring, which is monitored optically. The images obtained are critically dependent on the pressure, or force acting or applied, between the tip and the sample. Furthermore, optimal imaging conditions are inevitably sample dependent.

Whilst the AFM is important for imaging investigations, quantifying the tip-sample interaction has become increasingly important in order to improve the quality and reliability of images obtained. However, it was realized in 1991 that the AFM could be used to measure interaction forces directly between a small sphere, attached to the cantilever, and a flat substrate, resting on the piezoelectric positioner, forming an interesting and highly flexible adjunct to the conventional surface forces apparatus (SFA). Force-distance profiles can now be readily obtained for a variety of soft and hard interfaces and the "colloid probe" technique, as it has become widely known, has also been extended to the measurement of friction forces.

The technique is widely used in a large number of research laboratories, in industry, universities, and research institutions. The purpose of this IUPAC project is to produce a timely technical report that recommends experimental procedures for performing

colloid probe surface force measurements, in normal and lateral (frictional) modes. This project commenced in 2001 and is now in its final stages, with a second draft report prepared. The project team consists of John Ralston (University of South Australia, Adelaide, Australia), Ian Larson (Victoria College, Australia), Mark Rutland and Adam Feiler (Institute for Surface Chemistry, Stockholm, Sweden), Per Claesson (Royal Institute of Technology, Stockholm, Sweden), and Mieke Kleijn (Wageningen, Netherlands).



AFM—how to best obtain reliable images?

The second draft report, now in circulation, deals with the following:

- AFM development
- calibration of cantilever spring constant for normal (z) deflection
- calibration of piezoscanner
- colloid probe attachment
- force measurements
- construction of force versus distance curves
- different materials
- latest developments

A section on frictional forces is presently being expanded.

The penultimate report will be completed by late December of this year at which time a project meeting will be held in Adelaide to agree on the final version.

For more information, contact the Task Group Chairman John Ralston <[john.ralston@unisa.edu.au](mailto:john.ralston@unisa.edu.au)>.

 [www.iupac.org/projects/1999/1999-016-3-100.html](http://www.iupac.org/projects/1999/1999-016-3-100.html)

## Ionic Strength Corrections for Stability Constants

Version 1.5 of the Specific Interaction Theory (SIT) program was released this past September. The program uses specific interaction theory to render ionic strength corrections for stability constants, and includes activity coefficient calculation molar-molal interconversion. The SIT program can be readily applied to industrial processes for which stability constants may be required at very high ionic strengths.

The calculations of stability constants over a wide range of ionic strengths are not trivial, and require for instance a database of ionic coefficients for each ion-ion interaction. The program, developed by L. D. Pettit of Academic Software and part of this IUPAC project, performs the following:

1. calculates activity coefficients (0–5 m)
2. corrects stability constants for the general reaction:  $xM + yL + zH_2O$
3. calculates SIT(complex) values from sets of log K/ionic strength values
4. interconverts molarities - molalities
5. interconverts log K(molar) - log K(molal)

The user can select any of 14 background electrolytes and the program uses a text file which currently holds over 360 SIT parameters. The program has an extensive Help file that gives references and equations used. A Russian version, written by Dr. I Sukhno and Dr. V. Buzko, is now available.

Interested persons are invited to download this free program (see Web address below), test it, and send comments.

A comparable program to perform calculations using Pitzer parameters is being prepared. This will perform similar calculations to the SIT program and will also include activity and stability constants changes as a function of salinity, and oxygen, nitrogen, and carbon dioxide solubility as a function of salinity and fluid composition.

For more information, questions, and comments, contact the Task Group Chairman L. D. Pettit <[pettit@acadsoft.co.uk](mailto:pettit@acadsoft.co.uk)>.

 [www.iupac.org/projects/2000/2000-003-1-500.html](http://www.iupac.org/projects/2000/2000-003-1-500.html)