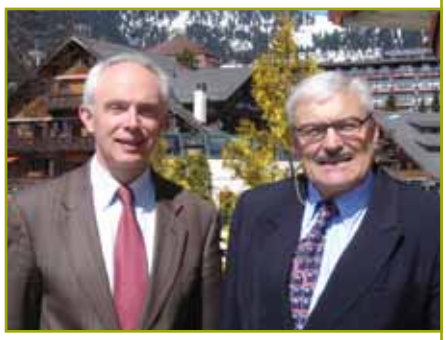
Where Does IUPAC Stand with Regard to this Discipline?

by Christopher Brett and Michel Rossi

The aim of the Physical and Biophysical Chemistry Division (PBCD), Division 1, is to organize and promote the international collaboration between scientists in physical and biophysical chemistry and related fields in accordance with the strategic goals and aims of IUPAC. More specifically it seeks to:

- address problems and formulate recommendations on nomenclature, symbols, units, terminology, and conventions in physical and biophysical chemistry, disseminate the recommendations, and encourage their translation as well as monitor their acceptance by the chemical community
- establish and stimulate the use of methodologies, standards, and reference materials in physical and biophysical chemistry
- encourage the compilation and documentation of critically evaluated physical chemical data
- recognize new developments in physical and biophysical chemistry and the fields in which they are applied
- promote future-oriented projects that contribute to science and technology and to the needs of the world community

These activities are carried out through PBCD projects and interdivisional projects, some of them involving the organization of special symposia. The Division Committee is currently composed of 10 titular members, 6 associate members, and 8 national representatives. The division committee meets every year, at the General Assembly in odd-numbered years and at a convenient location in even or "off" years, with regular contact between committee members by e-mail. The purpose of these meetings is to discuss current and completed projects, and to discuss strategy and possible new projects involving emerging themes of research on which consensus is needed, and that might be appropriate for the division. The membership of the committee is composed to ensure global diversity and expertise in most areas of knowledge and current activity within physical and biophysical chemistry, including thermodynamics, kinetics, theoretical chemistry, electrochemistry, surface and interfacial chemistry, and spectroscopy and all of its biophysical implications. Topics are addressed at the molecular level, in nanoscience, nanotechnology, and materials, and with links to energy, environment, and health.



Christopher Brett (left) and Michel Rossi.

The division is also home to the Commission on Physicochemical Symbols, Terminology, and Units, whose primary role is producing the "Green Book" (more details below). In addition, the division's Advisory Subcommittee, consisting of 44 distinguished scientists, helps to review project proposals and suggests themes for new projects. It has been very valuable in furthering division activities.

Twenty-one PBCD projects are currently under way, including four interdivisional projects and three that are nearing completion; the division is also participating in nine interdivisional projects led by other divisions. The large number of interdivisional projects testifies to the high importance given to the interdisciplinary nature of chemistry and to the strong links between physical and biophysical chemistry and other areas of chemistry. The traditional frontiers between the different "classical" areas of chemistry seem to become more fuzzy as we have recently seen an increasing number of project proposals that are addressed to several divisions at the same time. New materials, chemical applications directed to energy generation and storage, and the physical chemistry of nanoscience are just three examples of a possible paradigm change, perhaps at the expense of "traditional" biophysical or molecular/biochemical aspects in physical chemistry. We certainly will

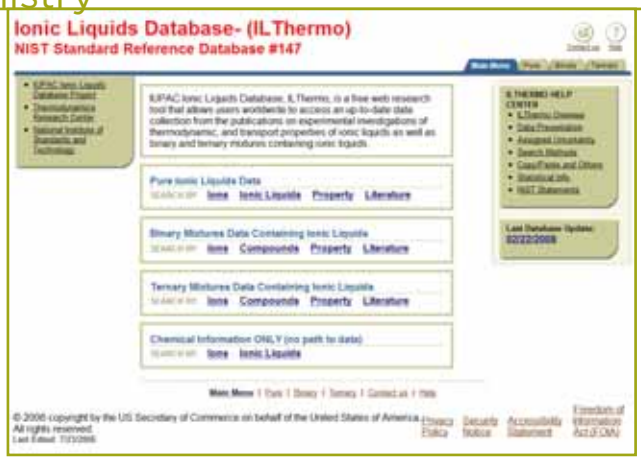
critically and continuously observe such developments in order to monitor subtle changes in the interest of the physical chemistry community at large.

Many of the division's projects have resulted in publications even before completion of the project, and new and ongoing projects have been described in articles in *Chemistry International*. Projects leading to technical reports on different topics, recommendations on the use of techniques and data analysis, and reporting and databases of critically-evaluated data have been produced. Each project has a member of the division committee attributed as a project monitor who acts as a liaison between the task group leader and the Division Committee.

Four examples are presented below that illustrate some of the current division activities, which, it is hoped, have a positive impact for chemists worldwide.

Over the last 10 years, an evaluated kinetic database with data relevant to atmospheric kinetics has been produced (see Tools of the Trade, Jan 07 *CI*, p. 15), together with a website <www.iupac.org/projects/2007/2007-001-2-100.html> and <www.iupac-kinetic.ch.cam.ac.uk>. This database has been highly successful, with a very large number of accesses, probably because of its impact on the simulations of climate change that take into account modifications of the composition of the atmosphere owing to chemical or photolytic reactions. In addition, selected rate constants also control the multiphase sulphur chemistry, simultaneously taking place both in the gas, as well as in the aqueous phase, of the ocean. Continuous updating is necessary and the protocols for future updating and addition of new reactions have been recently decided. Expansion of the atmospheric degradation reactions of organic compounds to include higher alkanes, aromatics, and perfluoro-compounds is being undertaken.

The division's projects involving ionic liquids arose as a result of the perceived need by the chemical community for better understanding of the thermodynamic and thermophysical properties for applications in industrial processes. In addition, there was interest in creating an open-access, free, and comprehensive online database for the storage and retrieval of metadata and numerical data in this new area, including the syntheses, structure, properties, and uses of this data.



Industrial applications are already emerging from this work. Details on the projects can be found at <www.iupac.org/projects/2002/2002-005-1-100.html> and <www.iupac.org/projects/2003/2003-020-2-100.html>. The ILThermo website (screen shot above) with ionic liquid data was officially launched in March 2006. It can be accessed at <ilthermo.boulder.nist.gov>. The site is divided into pure ionic liquids, binary and ternary mixtures, and further chemical information.

Another recent, important division activity was the publication of the third edition of *Quantities, Units and Symbols in Physical Chemistry* (Green Book) in July 2007 (see Nov-Dec 2007 *CI*, p.28). A project has just been approved to produce an abridged version of the Green Book in order to reach a wider audience, particularly students. Such an abridged version is necessary given the crucial importance of standardized nomenclature to enable proper communication of comparative data and to ensure standardized links between nomenclature and concepts. Translations of the Green Book into several other languages are planned, which attests to the great popularity of previous editions among students and professionals alike. Following IUPAC policy in this matter, management of the project and financial support will arise mainly from the concerned national chemical societies .

A final example concerns an innovative type of project with an educational slant that has just commenced. In conjunction with the Committee on Chemistry Education, this "test case" project seeks to reach out to parts of the world where resources are limited. The project involves promoting the application of

wet surface vibrational spectroscopies to problems in interfacial chemistry by selecting, documenting, testing, and disseminating to universities a collection of experiments, suitable for undergraduate teaching laboratories, that can be performed with inexpensive equipment. More details can be found at <www.iupac.org/projects/2006/2006-050-3-100.html>.

The increasingly interdisciplinary nature of chemistry, among its branches and between chemistry and other sciences and with engineering, is reflected in the division's close contacts with other IUPAC divisions and with Standing Committees. Such collaborations are expected to increase.

Last year's meeting of the Physical and Biophysical Division took place at the General Assembly in Torino in August 2007 with 11 members of the Division Committee present and three Young Observers who played an active part in the proceedings. One of the Young Observers has since submitted a project that is now underway. The Division Committee's 2008 meeting took place in April in Switzerland.

We are always seeking to identify and encourage project proposals, which should reflect the needs of chemistry today. These needs are in constant change, reflecting the needs of the chemistry community. For this reason, it is important that the Advisory Subcommittee advises us on new directions that members of the Division Committee may be unaware of.

If you feel that you can make a positive contribution to the work of the division and have an idea for an appropriate project, or have any other comments, please contact us via email at the addresses below.

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Stamps International

See also www.iupac.org/publications/ci/indexes/stamps.html

Triads, Triads, Everywhere

Johann Wolfgang Döbereiner (1780-1849), a professor of chemistry at the University of Jena, was the first to recognize that several groups of three elements, such as lithium, sodium, and potassium, or chlorine, bromine, and iodine, had similar chemical properties. In addition, he noticed that the atomic weight of the middle element in these triads was roughly the average of those of the other two. These observations led to his Law of Triads (1829), which firmly established his reputation as a pioneer in the development of the modern periodic table some 40 years before Mendeleev's masterpiece was published.

However, the stamp illustrated in this note, issued in East Germany (DDR) on 26 February 1980 to commemorate the 200th anniversary of Döbereiner's birth (which was actually on 13 December 1780), does not mention his seminal contribution to the organization of the elements but features instead his "other" claim to fame. The stamp shows a schematic drawing of his renowned lighter, in which a stream of hydrogen gas, generated from zinc and sulfuric acid, spontaneously ignites upon contact with finely divided platinum. This

novel chemical reaction received a lot of attention since it was first described by Döbereiner in the summer of 1823 and was swiftly reproduced by others. Within months the discovery was reported in multiple European scientific journals, which ushered in an era of interest in catalysis that continues to this day.

For a recent discussion of triads in the periodic table, see: Scerri, E. *J. Chem. Educ.* 2008, **85**, 585-589.

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