PHYSICAL AND BIOPHYSICAL CHEMISTRY DIVISION REPORT
FIRST YEAR OF THE BIENNIUM 2004-2005

SEPTEMBER 2004

REPORT TO THE IUPAC BUREAU: MEETINGS IN BLED, SLOVENIA OCT 2004

Executive Summary and Highlights

The change in name of Division I in autumn 2000 to Physical and Biophysical Chemistry Division (PBPCD) has led to initiatives to promote projects from those working in the **Biosciences subject area**. A major international workshop on the Physical Chemistry of Biointerfaces was held near Adelaide, South Australia 23–26 May 04 in series with the Seventh World Biomaterials Congress in Sydney, Australia 17-21 May 04. IUPAC was well represented with the Past President of Division I being one of the organisers of the workshop attended by the current President of the Division. Time was set aside for these two individuals to address the attendees about the IUPAC system for funding support and to encourage the submission of projects. The workshop was aimed at providing fundamental insights into topics such as interfacial forces and properties involved in protein/surface interactions and the molecular kinetics of drug delivery. The workshop itself was very successful and we wait to see its success in encouraging IUPAC participation. It is clear that there is a need for standardisation of terminology and agreement on calibration protocols, both areas where IUPAC can play an important role as the catalyst.

The Division continues with its important work of **establishing databases in specific subject areas**. A significant advance has been achieved with our project of evaluated kinetic data for atmospheric chemistry by setting up a website at the University of North Carolina, USA, to mirror the parent site in Cambridge, UK. The site continues to attract some 2000 accesses per week. A substantial number of downloads continues in areas of heterogeneous reactions, thermodynamic data and in guides to the data sheets. The positive spin off is being realised from the decisions taken at the Bureau meetings in Paris to locate all the databases at the University of North Carolina with service support from the IUPAC secretariat and maintenance from the Division. It is at the stage of submission of a project proposal that these matters are to be defined clearly.

The Division remains active with its **chemical thermodynamics** component. You will recall that as a result of the IUPAC restructuring beginning in 2002, the International Association of Chemical Thermodynamics [IACT] was set up. The IUPAC Council at its meeting in Ottawa in August 2003 granted the IACT Associated Organisation status within IUPAC. The IACT has held its biennial meeting, the 18th IUPAC International Conference on Chemical Thermodynamics, in Beijing, P.R. China, during August 2004 with an especially large attendance by scientists from within Asia. Topics areas include electrolytes and non-electrolytes, new materials, supercritical fluids, biological applications, medical applications, interfaces, molecular simulation, energetics, industrial thermodynamics and databases, and frontiers in thermodynamics.

The Division is contributing to the final stages of **the revision of the Third Edition of the Green Book [Quantities, Units and Symbols in Physical Chemistry**], through its membership in the IDCTNS. The third edition is to be placed in whole or in part on the Web as well as to be translated into several languages. For the biennium 2005-06, the Division has 28 projects underway of which 8 are nearing completion and 5 are interdivisional. This total of 28 compares with 35 for the 2003-04 biennium as the Division attempts to focus its efforts on fewer projects but with more financial support for each.

The initiative by the Division to establish **the Advisory Subcommittee of 61 international distinguished scientists and engineers**, some of whom are drawn from industry, is bearing fruit. The members of the subcommittee are listed on the IUPAC website and in the IUPAC Handbook (p29) and all are IUPAC Fellows. The role of the subcommittee is to serve as a sounding board for the Division Committee, suggesting areas that may by dealt with by the Division, drawing attention to the need for experimental protocols in specific subject areas, taking part in IUPAC conferences, and acting as one source of expert referees for IUPAC proposals. The immediate benefit realised from the subcommittee is the reduction of the period needed for the assessment of project proposals to a period of weeks rather than months. It is important to realise that the responsibility for leading and guiding the Division to include encouraging and supporting all its growing activities lies on the shoulders of a relatively few individuals who also have heavy responsibilities in their work place and who undertake IUPAC work for public service and service to their profession. The network created by the establishment of our Advisory Subcommittee has been helpful in this regard as well as by the IUPAC Secretariat. The membership of the subcommittee is to be reviewed biennially.

Activities of Division I within the IUPAC Framework and its Goals

In their totality, the projects of Division I embody all of the five long-range goals of IUPAC. Some projects support certain goals more strongly than other projects depending on the nature of the project. In terms of **leadership**, the Division continues to exert a strong role through the Interdivisional Committee on Terminology, Nomenclature and Symbols. Its current major project is the production of the new edition of the Green Book, whose influence is very significant in education, research, industry, and publishing through the world. The Division's work with the Chemical Education Committee serves both goals of **leadership** and **chemical education**. Its projects through the International Association of Chemical Thermodynamics promotes connections to **chemistry-related industry** via workshops, **communications** among individuals and the addressing needs of chemistry and applied chemistry in **developing countries** via the rotation of conferences to include these countries with special financial incentives to assist attendance. Several of the Division's current projects are devoted to **advancing research in the chemical sciences** via international **standardisation**, while simultaneously promoting **scientific discussion**.

The creation of the 61-person Advisory Subcommittee has **broadened the membership base** of the Division significantly with a geographic balance and with an attempt to address the gender and age imbalance.

The following list contains the 15 Current Projects, the 8 projects nearing completion, the 5 other interdivisional projects and the four projects in review at the time of preparing this report.

A. CURRENT PROJECTS

1998-130-32 – Electrochemistry at the interface between two immiscible electrolyte solutions*

1999-037-2-100 - Evaluation kinetic data for atmospheric chemistry

2000-002-2-100 - Standardization of methods for the characterization of inorganic membranes*

2001-015-1-100 - Standard potentials of radicals*

2001-028-1-100 - Electrochemical impedance spectroscopy - terminology, nomenclature and data exchange formats

2001-030-1-100 - Recommendations on the measurement and analysis of results obtained on biological substances with isothermal titration calorimetry

2001-035-1-100 - Measurement and interpretation of electrokinetic phenomena

2002-005-1-100 - Thermodynamics of ionic liquids, ionic liquid mixtures, and the development of standardized systems

2002-063-1-100 - Chemical thermodynamics in industry. (2004-029-1-100 Extension of 2002-063-1-100).

2003-005-1-100 - Recommended values of the viscosity of molten iron and aluminum

2003-006-1-100 - NMR chemical shifts: updated conventions*

2003-020-2-100 - Ionic liquids database

2003-024-1-100 - Selected free radicals and critical intermediates: thermodynamic properties from theory and experiment

2003-036-2-100 - Thermodynamics and non-equilibrium criteria for development and application of supplemented phase diagrams

2004-010-3-100 – Heat capacity of liquids: critical review and recommended values for liquids with data published between 2000 and 2004.

2004-021-1-300 - Reference Methods, Standards, Applications of Photoluminescence.*

2004-028-1-700 - Practical studies for medicinal studies. An integrating approach for developing countries.*

* Interdivisional project

B. PROJECTS NEAR COMPLETION / IN PRESS

110/2/81 - Revision of "Quantities, Units and Symbols in Physical Chemistry" and the Appendices (3rd edition)

120/15/95 - Thermochemistry of chemical reactions: nomenclature, symbols and experimental methods for bond energies.

120/16/97 – New edition of Experimental Thermodynamics Volume II

150/24/95 - Spectroscopy under extreme conditions of temperature and pressure

1999-016-3-100 - Recommendation for the use of AFM in the direct measurements of colloidal forces

2002-008-1-300 - Chemical actinometry*

2000-026-1-100 - Critical compilation of vapour liquid critical properties

2004 IUPAC Technical Report (Pure & Applied Chemistry in press) – Standards, calibration and guidelines in microcalorimetry: Part 2. Calibration standards for differential scanning calorimetry. (Della Gatta, Richardson, Sarge, Stolen).

C. OTHER INTERDIVISIONAL PROJECTS

2000-012-1-300 - Single molecule spectroscopy

2001-036-1-300 - Glossary of terms in photocatalysis and radiation catalysis

2002-024-1-300 - Glossary of terms used in photochemistry (3rd version)

2003-056-2-500 - Standard definitions of terms relating to mass spectrometry

2004-021-1-300 - Reference methods, standards and applications of photoluminescence

D. PROJECTS IN REVIEW

2004-022-1 – Terminology and measurement techniques of starch componenets (IRRI Ref DPPC2004-21)*.

2004-026-1 – Defining the hydrogen bond.

2004-027-1 – Evaluated kinetic data for atmospheric chemistry.

2004-028-1 – Practical studies for medicinal studies. An integrating approach for developing countries.

* Interdivisional project