

# PHYSICAL AND BIOPHYSICAL CHEMISTRY DIVISION

## DIVISION 1

### SUMMARY REPORT

September 2006

The objective of this report is to briefly summarise activities during the past year and, in particular, to give an update on developments since the Division Committee Off-Year Meeting in April 2006. Besides the Division Committee, the division has one commission: Commission I.1 "Commission on Physicochemical Symbols, Terminology, and Units" and an Advisory Sub-Committee, currently with 42 members.

#### **Off Year Meeting, April 2006**

The Off-Year Meeting was held in Coimbra, Portugal from 8-9 April 2006. It was attended by 7 TMs and 1 AM, together with the President of IUPAC. The minutes of the Meeting are on the web and can be consulted for details.

#### **Current Projects**

A list of the current projects - databases, recommendations and technical reports - is annexed and all are proceeding well with acceptable and justified deviations from the timeline. Many of these are large-dimension projects. Members of the Division Committee act as monitors for all divisional projects as well as liaison for interdivisional projects. Some projects are leading to web pages and some to publication in journals such as for example, J. Phys Chem. Ref. Data.

#### **New projects**

A new project has just been approved: "Liquid Intrusion and Alternative Methods for the Characterization of Macroporous Solids".

A project "Recommendations for nomenclature and databases for biochemical thermodynamics" is in the final stages of the approval process.

Two other projects in the areas of vibrational spectroscopy and theoretical chemistry are expected to be submitted very shortly.

A new project proposal on atmospheric kinetics will be submitted in 2007, after the present project is completed, and other proposals are expected.

#### **"Quantities, Units and Symbols in Physical Chemistry" and Appendices (3rd edition)**

The electronic version of the Green Book finished its period of public review on 31<sup>st</sup> March 2006. Many comments were made and it was necessary to hold a meeting of Commission I.1 in Zurich

from 18-20 August to sort out the final open points. Final proof-reading has been completed and indexing is being done. It is expected that submission to RSC will be in the second half of October.

### **Dissemination of divisional activities**

Apart from dissemination in PAC, journals and on web pages, PBCD is presently contributing two articles on the atmospheric kinetics and ionic liquids projects to the series of articles “Tools of the Trade”, in *Chemistry International*.

### **Biophysical Chemistry**

Following the Off-Year Meeting, a thorough investigation of the possible contributions that the Division can make, is being undertaken, including IUPAC sponsored sessions at a Biological symposium or conference.

### **Commission I.1**

The primary task of Commission I.1 has been the preparation of the 3<sup>rd</sup> edition of the “Green Book”. Now that this will be soon completed they will look towards other projects in this area such a web-based version of the Green Book and a “reduced” version for undergraduates and schools.

### **Elections**

The Nominating Committee has been formed with Prof. Ron Weir (Past President) as chair. Its composition has been approved by the Secretary General. It was agreed that the Nominating Committee will seek to cover all the key areas of physical and biophysical chemistry in the Division Committee membership.

### **IUPAP**

Prof. R. Lynden-Bell (Div. Secretary) has agreed to serve in Commission C3 on Statistical Physics of IUPAP, as Associate Member, to reflect the strong relation between statistical physics and physical and biological chemistry.

Christopher Brett  
30 September 2006

## Annex:

### Current projects

- 1999-037-2-100 - Evaluation kinetic data for atmospheric chemistry
  - 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
  - 2002-005-1-100 - Thermodynamics of ionic liquids, ionic liquid mixtures, and the development of standardized systems
  - 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
  - 2004-026-2-100 - Categorizing hydrogen bonding and other intermolecular interactions
  - 2004-035-1-100 - A database of water transitions from experiment and theory
  - 2004-036-1-100 - Establishing recommended data on thermodynamic properties of hydration for selected organic solutes
  - 2005-016-1-100 - Developments and applications in solubility\*
  - 2005-048-2-100 - Solubility and thermodynamic properties related to environmental issues\*
  - 2006-021-2-100 - Liquid intrusion and alternative methods for the characterization of macroporous solids
- \* Interdivisional project

### 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
- 2004-005-2-500 - Comparable pH measurements by metrological traceability
- 2004-021-1-300 - Reference methods, standards and applications of photoluminescence
- 2005-042-1-300 - Chemistry for Biology - an inventory of interdivisional and interdisciplinary activities within IUPAC in the field of biological chemistry

### 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
- 150/24/95 - Spectroscopy under extreme conditions of temperature and pressure
- 2000-026-1-100 - Critical compilation of vapour liquid critical properties