

PHYSICAL AND BIOPHYSICAL CHEMISTRY DIVISION REPORT

2002-2003 BIENNIUM

JUNE 2003

Executive Summary and Highlights

The Physical and Biophysical Chemistry Division [PBPCD, Division 1] has now moved into a project-based organization that is completely different from the past IUPAC Structure. In September 2000 the name of the Division was changed to embrace Biophysical Chemistry, recognizing that **many areas of bioscience are underpinned by physical chemistry**. Whilst this is a new area of activity for the Division, it is pleasing to see that the Division has been actively involved in an innovative conference on Biophysical Complexity, held in Southampton in April of this year. One successful aim of the meeting was to actively engage young researchers in the early stages of their research careers. An outstanding group of plenary speakers took part, drawn from Departments of Chemistry, Medicine, Bioengineering, Cell Biophysics, Anthropology and Human Genetics, among others. Dr Jeremy Frey represented the Division at this highly successful meeting. A Report will be published in Chemistry International in the near future. A major international workshop on the Physical Chemistry of Biointerfaces will be held in the Barossa Valley near Adelaide, South Australia from May 23 to May 26, 2004. This is a satellite workshop that will be held immediately following the Seventh World Biomaterials Congress [Sydney, Australia, May 17-21 2004]. The Division President is one of the organizers. This workshop is 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, to give just two examples. Advances in materials science, molecular biology, surface and interface analysis methods and theoretical and modelling approaches to biological systems will be key foci. It is intended that this workshop will be supported in part by IUPAC as an innovative conference under the banner of New Directions in Chemistry. Additional support is anticipated from private industry and from the Australian Government. These two Biophysical Chemistry initiatives were outcomes of an important debate which commenced at the Division's off-year meeting in Morges, Switzerland in April 2002 and continued in Paris at the Maison de la Chimie Bureau Meeting the following September. They are the harbingers of future larger scale activities in this area of Biophysical Chemistry by the Division.

The Division's **very important work in establishing databases** in key areas continues. Of particular importance is our work on evaluated kinetic data for atmospheric chemistry. The website development has been very sound and there is now a mirror site at the University of North Carolina as well as the parent site in Cambridge. The site attracts about 2000 accesses per week, a very respectable figure indeed. Substantial numbers of downloads occur in areas covering heterogeneous reactions, thermodynamic data and guides to data sheets. As well as this there are over 300 subscriptions to the mailing list for announcements. The important issue of database management was dealt with sensibly at the Paris Bureau meeting, by a small task force that included the President of the Division. All databases will be physically located at the server in North Carolina from the outset of the project. The secretariat will provide service whilst maintenance will be the responsibility of the Division- both will be addressed at the proposal stage for any project. Presently a significant proposal to develop a database for ionic liquids, whose development was actively encouraged by this Division [commencing at the Morges off-year meeting], is being assessed for support, so that it is very pleasing indeed to see that the vexed question of database management has been settled.

The Division has been **very active in chemical thermodynamics** for many years. Following the restructuring of IUPAC at the end of 2001, the International Association of Chemical Thermodynamics [IACT] was established and, in April 2003, the IUPAC Executive recommended that the IACT be granted Associated Organization status within IUPAC, and that this recommendation be approved by Council at the August meeting in 2003. The IACT has been very active, covering topics as diverse as electrolyte solution data and microcalorimetric standards to new areas such as the thermophysical properties of polymers. It is heartening indeed to see that this important Divisional area is vibrant and active.

The Division is actively contributing to the final stages of the **revision of the Third Edition of the Green Book** [Quantities, Units and Symbols in Physical Chemistry], through membership of ICTNS. It is expected that this Third Edition will in part or in total be placed on the Web and also translated into foreign languages. Of the **23 listed projects for the Division, 7 are near completion** or in press. We have seen an **intentional decrease in the number of active projects from the previous biennium**, when 35 projects were underway. There has been a conscious effort by the Division to complete projects and also to focus on larger, better resourced activities that can be completed within acceptable time frames. It is notable that seven projects are interdivisional, a clear demonstration of the key central role that the Division plays in Chemistry.

An important initiative by the Division has been **the establishment of an Advisory Group of 61 international distinguished scientists**, a small proportion of whom are drawn from industry. The membership is listed on the IUPAC website. The role of this Advisory Group is to act as a sounding board to the Division Committee, suggesting areas that might be dealt with by the Division, drawing attention to the need for experimental protocols in certain areas, taking part in IUPAC conferences and acting as one source of critical referees for IUPAC proposals. One pleasing outcome of this Advisory Board is that the project assessment period for new proposals has been shortened considerably, to periods of often just several weeks. One needs to recognize that the responsibility of guiding the Division and encouraging all activities now rests on the shoulders of a rather small number of chemists, most of whom are very active researchers with heavy responsibilities. Networks of "IUPAC sensitive" scientists are invaluable in terms of support, as is the superb role played by the Secretariat. The membership of the Advisory Group will be reviewed on a biennial basis.

In terms of **succession planning**, it is important to note that the current President and Vice President of the Division will be retiring from IUPAC at the end of 2003. Office bearers for 2004-2005 have been nominated and the process of electing new members is now well-advanced.

Activities Within the IUPAC Framework and Its Goals

In connection with leadership in the area of nomenclature and terminology, the PBPCD has taken a very substantial role through the creation of the Interdivisional Committee on Terminology, Nomenclature and Symbols, with Dr J. Frey as Chair. The principal responsibility of this Committee has been the revision of the Green Book, now almost complete. The Division has strengthened its ties with industry through the creation of an Advisory Group having industry representation as well as involving industrial scientists in IUPAC- sponsored conferences and workshops run by and/or linked to the Division. In the area of database creation and management the Division has always been very active and will continue to do so. Present examples include its important work on atmospheric chemistry and the forthcoming project on ionic liquids. For some years the Division has organized major conferences dealing with environmental problems [e.g Interfaces Against Pollution] and will continue to support this activity.

Through the maintenance of its very strong science base and cordial interactions, the Division's excellent links to the Committee on Chemistry Education will continue to be sound. The Division is now making its presence felt in Biophysical Chemistry-related activities, focussing on international conferences and workshops at the outset. This serves multiple purposes- raising the profile of IUPAC in this multidisciplinary domain; helping define areas where standards, databases, protocols etc may be necessary; and producing worthy publications under the IUPAC banner.

The Division **continues to encourage**, engage and **involve younger researchers** wherever possible. This may be through the various formal IUPAC schemes [e.g. Young Observer program], but also through projects where the project team is constructed so that young researchers can contribute strongly. In this context it is important that the project be well focussed, with clear targets and a relatively short [a few years at most] time horizon. The Advisory Group is playing a useful role in the commencement of new projects, an activity that needs to be nurtured and expanded if the Division is to remain active and strong in the coming years.

In terms of projects and focus, the Division's present activities embrace spectroscopy and photochemistry, photocatalysis, kinetic data for atmospheric chemistry, membrane characterization, electrochemistry and electrokinetic phenomena, the measurement of colloidal forces using atomic force microscopy, standard potentials of free radicals, thermodynamics and NMR chemical shift conventions. **Several major activities are now summarised, followed by several smaller project summaries.** All projects are monitored by at least one member of the Division Committee and a major review will take place in August of this year.

The International Association of Chemical Thermodynamics (IACT) was established following the restructuring of IUPAC at the end of December 2001, in order to continue the work of the former Commission I.2 on Thermodynamics. Its objective is to maintain the highest standards in teaching and research in this key area of chemistry, chemical engineering, materials science and the biosciences. In order to maintain close links with IUPAC, application was made for Associated Organization status within IUPAC. In April 2003, the IUPAC Executive Committee recommended that this be approved by Council at its meeting in August 2003.

The major activities of IACT include the following:

1. To plan the biennial IUPAC International Conferences on Chemical Thermodynamics (ICCT).

Arrangements for ICCT-2004 in Beijing are proceeding according to our Guidelines for Organisers, but in view of the problem with SARS, a discussion on the suitability of the venue location will be taking place at the IACT Board meeting in Boulder, Colorado, USA, 22 June 2003. The ICCT-2006 is planned to be held in Boulder, Colorado.

2. To encourage collaboration with continuing projects, which are:
 - a. Electrolyte Solution Data;
 - b. *Project on the Thermochemistry of Chemical Reactions;
 - c. Standards, Calibration and Guidelines in MicroCalorimetry; Vapour Liquid Critical Properties of Elements and Compounds;

- d. *International Thermodynamic Tables of the Fluid State. Benzene;
- e. *New edition of Experimental Thermodynamics Volume VI. Measurement of the Thermodynamic Properties of Single Phases : Editors: A.R.H. Goodwin, K.N. Marsh and W.A. Wakeham and Volume VII. Measurement of the Properties of Multiple Phases: Editors: Th. W. de Loos and R.D. Weir; Ionic Liquids (K.N. Marsh);
- f. *Chemical Thermodynamics in Industry;
- g. *Recommended values for the viscosity of molten iron and aluminium.

[* Division I Projects]

3. To propose relevant new projects, for example:

- a. XML based IUPAC Standard for Thermodynamic Property Data Capture and Storage (to be revised);
- b. Thermophysical properties of polymers: to include DfH, Tf, glass transition temperatures and thermo-mechanical coefficients over extended temperature and pressure ranges;
- c. Guidelines for temperature modulated DSC.

Our database work in atmospheric chemistry is continuing at a high rate. **In the case of our Evaluated Kinetic Data for Atmospheric Chemistry, substantial progress has been made on the first phase (July 2001-July 2003)** of the IUPAC funded project to develop a website containing the evaluated data. The work covers development of a linked, interactive website, retyping and posting of new updated data sheets and other information relating to the evaluation, and creation of a mirror site at the IUPAC HQ website in North Carolina.

On the website development the progress has been good. The structure has been improved to make addition of new data sheets more flexible. All the data sheets for reactions of Ox, HOx, NOx and SOx reactions, and most of the organic reactions updated by the Task Group in the past 2 years have now been added. The summary sheet has been updated as new data sheets are added, and supplementary material posted on the site. Links have been introduced to link the summary sheet to specific data sheets. The remaining work for this year is to incorporate the updated data sheets for the halogen species.

Web traffic has stabilised over the past months and the current number of accesses (about 2000 per week) is very pleasing. The web server logs also give an indication of what is the most popular download. In a typical week, of the 2200 connections in that week, some 300 are to the main page and there are about 1000 downloads of the IUPAC summary. The introductions to the reactions are proving rather popular. There are 50 downloads of the introduction to heterogeneous reactions, downloads of the PDF on thermodynamic data and 20 downloads of the "guide to data sheets" in a typical week.

There are currently 311 subscriptions to the mailing list for announcements. Unlike the website statistics this is the most accurate measure of interest in the site and continues to increase.

The mirror site at UNC is now operational. After considerable delays at the US end, access to the IUPAC mirror site was finally obtained in 2002. Prior to copying the IUPAC website files to the US site a number of changes had to be made to the master IUPAC site in Cambridge. These were necessary to remove any references to the Cambridge site and make all links within the pages relative rather than referring to absolute directory names. The directory structure is somewhat different on the US side and in future all new pages must use relative links to make sure they will work correctly.

The SQL database has been set up on the US site and all web pages have been copied over. However, there are no links to the site from the Cambridge site nor from the main IUPAC site as yet but this should be in place soon. The remaining issue to sort out is how to allow updating of the website and making sure the two sites are consistent with each other.

In terms of smaller projects, two examples are indicative of the general activity. **For Electrochemical Impedance Spectroscopy**, an extensive draft report has been prepared which covers all the subject matter and is now under discussion by members of the project task group as well as being circulated to other selected scientists and instrument manufacturers for comment. It is a concern to have as wide an agreement as possible, particularly on data exchange formats and presentation, since electrochemical impedance is currently used by scientists and engineers in many different fields. Additionally, an ISO norm is currently being prepared regarding organic coatings on metals including characterization by impedance (one of the task group members is chairman of the ISO working group).

The project meeting originally planned for November 2002 did not take place owing to difficulties in timing between the 4 members of the task group, and will do so in the first half of this year.

The project **Recommendation for the Use of the AFM in the Direct Measurements of Colloidal Forces**, has progressed to the draft stage and the members of the project team are presently reviewing the material. A decision has been made to include friction forces as well as normal forces and additional material is now being prepared. Considerable debate is taking place regarding the best way to deal with deformable interfaces [e.g. droplets, bubbles, blood cells], for this area should also be included. It is anticipated that the final draft will be complete by early November and members of the team will meet in mid December of this year to produce the final polished version. The Division's future activity in the Physical Chemistry of Bio-Interfaces is shown in the First Announcement, included as an Appendix to this report. This important area will grow in the future as part of the Division's broadening base.

The Division is presently in a healthy state of activity across a number of areas. For this to be maintained in the coming years, the composition of its members requires careful evaluation. For the Division to be credible, active researchers with strong international profiles should be recruited and, if they are to be effective they must be personally very energetic. Furthermore their networks must be strong and active, excellent assistance must be provided in their home Universities and/research institutions and, finally, the continuing support of a first rate secretariat is essential. IUPAC is an important organization and needs to have a much wider influence than it presently does. Membership of IUPAC Divisions needs to be seen as a career-enhancing activity, to which younger chemists should aspire.

John Ralston
President Division of Physical and
Biophysical Chemistry
June 2003

CURRENT PROJECTS

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

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

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

2000-013-1-100 - Selected free radicals and critical intermediates: thermodynamic properties from theory and experiment

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

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

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

* Interdivisional project

OTHER INTERDIVISIONAL PROJECTS

2000-012-1-300 - Single molecule spectroscopy

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

2002-008-1-300 - Chemical actinometry

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

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 Vol II

121/13/89 - International Thermodynamic Tables of the Fluid State, Volume 14 : Benzene

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

150/25/98 - Quantities, terminology and symbols in photothermal and related spectroscopies

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

RECENT PUBLICATIONS

Recent Reports

PHYSICAL AND BIOPHYSICAL CHEMISTRY DIVISION (I)

[Measurement of pH. Definition, standards, and procedures](#) (IUPAC Recommendations 2002) (V, I)
Pure Appl. Chem. **74**(11), pp. 2169-2200, 2002

[Definitions, terminology and symbols in colloid and surface chemistry](#)
(*Pure Appl. Chem.*, **31**, 579-638, 1972)
> Web Version 2001

[Heat capacity of liquids: Critical review and recommended values. Supplement I](#)

Milan Zábbranský, Vlastimil Ruzicka, Jr., and Eugene S. Domalski
Journal of Physical and Chemical Reference Data, **30**, No. 5, 1199-1689, 2001

[NMR nomenclature. Nuclear spin properties and conventions for chemical shifts](#) (I.5)

Pure Appl. Chem. **73**(11), pp. 1795-1818, 2001

[Standards in isothermal microcalorimetry](#) (I.2)

Pure Appl. Chem. **73**(10), pp. 1625-1639, 2001

[Quantum chemical B3LYP/cc-pvqz computation of ground-state structures and properties of small molecules with atoms of \$Z \leq 18\$ \(hydrogen to argon\)](#) (I.5)

Pure Appl. Chem. **73**(9), pp. 1521-1553, 2001

[Use of Legendre transforms in chemical thermodynamics](#) (I.2)

Pure Appl. Chem. **73**(8), pp. 1349-1380, 2001

[Nomenclature of Structural and Compositional Characteristics of Ordered Microporous and Mesoporous Materials with Inorganic Hosts \(IUPAC Recommendations 2001\)](#) (I.6)

Pure Appl. Chem. **73**(2), pp. 381-394, 2001

[Vapor-Liquid Critical Properties of Elements and Compounds: Part 8. Organic Sulfur, Silicon and Tin Compounds](#) (I.2)

Journal of Chemical & Engineering Data **46**, pp. 480-485, 2001

[Guidelines for presentation of methodological choices in the publication of computational results. B. Semiempirical electronic structure calculations](#) (I.5)

Pure Appl. Chem., **72**(8), pp. 1449-1452, 2000

[Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry. Supplement VIII \(Halogen Species\)](#) (I.4)

J. Phys. Chem. Ref. Data, 2000, 29, 167-266

[Pillared Clays and Pillared Layered Solids](#) (I.6)

Pure Appl. Chem., **71**(12), pp. 2367-2371, 1999

[Electrochemical Biosensors: Recommended Definitions and Classification](#) (I.7, V.5)

Pure Appl. Chem., **71**(12), pp. 2333-2348, 1999

[Interfaces Against Pollution](#) (I.6)

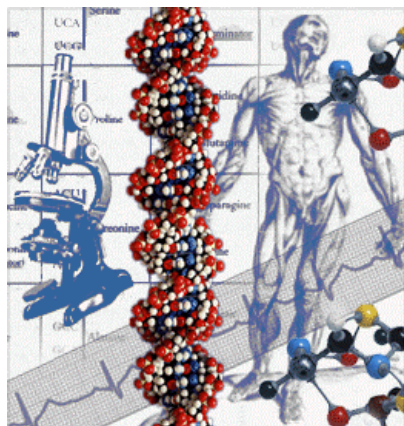
Colloids and Surfaces A, **151**, Nos. 1 and 2, 1999

International Conference & Workshop Physical Chemistry of Bio-Interfaces

Sunday 23rd May to Wednesday 26 May 2004
Novotel Barossa Valley Resort
South Australia, Australia

First Announcement

This workshop will focus on physico-chemical considerations of bio-interfaces. Held immediately following the 7th World Biomaterials Congress (17-21 May, 2004, Sydney, Australia), it is intended as a satellite workshop devoted to the study of bio-interfaces using physico-chemical methods and aimed at providing fundamental mechanistic insights, and to provide the opportunity for in-depth discussions



facilitated by the workshop format, on topics such as interfacial forces and properties involved in protein/surface interactions, non-fouling surfaces, molecular kinetics of drug delivery, and others. Invited and contributed talks will be selected for their ability to progress fundamental understanding relevant to biomaterials, bio-diagnostics and drug delivery applications.

This workshop will provide an interdisciplinary forum for the presentation and discussion of experimental and theoretical studies of bio-interfaces and biomolecule-surface interactions. Increased understanding of interactions between biomolecules and surfaces, the behaviour of complex macromolecular systems at materials interfaces, and biomolecule-biomolecule interactions, will contribute to the rapid growth in biomedical research, biotechnology, diagnostics, proteomics, genomics, dentistry and medicine. Advances in materials science, molecular biology, surface and interface analysis methods, and theoretical and modelling approaches to biological systems will feature in this workshop, as well as experimental tools and theoretical models to describe bio-interface phenomena with physical concepts and rules that allow predictive, model-driven research.

Program Outline

Sunday 23 May 2004	3.00 to 6.00pm 6.00 to 7.30pm Evening	Registration Welcome Reception Plenary lecture ("Setting the scene")
Monday 24th May 2004		Scientific Sessions Evening Poster Session
Tuesday 25th May 2004	Morning Afternoon	Scientific Sessions Tour of Wineries or leisure

Evening

Discussion session

Wednesday 26th May 2004

5.00pm

Scientific Sessions

Close of workshop

** Session titles and invited speakers will be detailed in the second announcement*

The Venue

The Barossa Valley is Australia's premier winemaking region. With a superb climate, large vineyards, towns that still reflect settlement by early 19th Century German immigrants and a typically relaxed South Australian lifestyle, the Barossa will charm the visitor.

Located just north of the city of Adelaide, it is easily reached from Adelaide Airport, which is served by National and International connections.

The Novotel Barossa Valley Resort is set in a natural amphitheatre, overlooking Jacob Creek and the North Para River in the heart of the Barossa Valley. Surrounded by picturesque vineyards with many famous boutique wineries to explore you can be guaranteed a warm welcome, superb facilities and the highest standard of service.



Organising Committee

Prof. Hans Griesser (Chair)	Ian Wark Research Institute, University of South Australia
Prof. John Ralston	Ian Wark Research Institute, University of South Australia
Dr. Clive Prestidge	Ian Wark Research Institute, University of South Australia
Dr. Joe Shapter	Department of Chemistry, Flinders University
Dr. Sally McArthur	University of Sheffield, UK

*** Additional Committee members will be detailed in the second announcement*

Further information and a call for contributions will be in the second announcement, due early August 2003.

Information on alternative accommodation and tourism options will be available from the Organising Committee.

For any queries, please contact either hans.griesser@unisa.edu.au or kathryn.prohaska@unisa.edu.au and use these email addresses to also notify us of your interest in receiving the second announcement.