IUPAC DIVISION I: PHYSICAL AND BIOPHYSICAL CHEMISTRY

REPORT TO COUNCIL: 2005-7

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I. EXECUTIVE SUMMARY AND HIGHLIGHTS

The Objectives of the Physical and Biophysical Chemistry Division, as stated on the Division web page, are to organize and promote the international collaboration between scientists in physical and biophysical chemistry and related fields in order to

- address problems and formulate recommendations on nomenclature, symbols, units, terminology and conventions in physical and biophysical chemistry, disseminate the recommendations, 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 its fields of applications; and
- promote future oriented activities important for the contribution of physical and biophysical chemistry to science and technology and to the needs of the world community.

The Physical and Biophysical Chemistry Division (PBCD) has continued its activities in both physical and biophysical chemistry, with regard to the aims of the division. The composition of the Division Committee is designed to cover all the different areas of physical and biophysical chemistry and identify topics in which the division can make new contributions.

For the biennium 2006-07, the Division has 26 projects running, which include five nearing completion and five interdivisional. This total compares with 28 for the 2004-05 biennium, representing a slight reduction as the Division continues to focus its efforts on fewer projects but with more financial support for each of them. These projects encompass different areas of physical and biophysical chemistry. Each project has a monitor who is a member of the Division Committee and is responsible for overseeing its running, if it adheres to the timeline and helping to solve any difficulties which may arise. Many of the projects have resulted in publications even before they are completed and new and on-going projects have been described in articles in Chemistry International. In general, dissemination of the results of projects is through web pages, Pure and Applied Chemistry and other journals such as J. Phys Chem. Ref. Data (see Publications in Section IV).

Details of the current state of the projects are to be found in Section III of this report.

Work on establishing databases has continued. Of particular note are those on evaluated kinetic data for atmospheric chemistry for which there is a website in the USA to mirror the parent site in Cambridge, UK. This is an on-going project for which a new project proposal has been recently submitted. A second database regards the new field of ionic liquids. This database was officially launched during the American Chemical Society Meeting in March 2006 and was well received.

The Third Edition of the Green Book [Quantities, Units and Symbols in Physical Chemistry], will be finally published at the end of July 2007, in time for the 2007 General Assembly. The Division has contributed to the final stages of its revision through its membership in the ICTNS. This new edition addresses many of the questions which were raised after the second edition. It is planned to place part or whole of the third edition on the Web and to translate it into several languages. Additionally, "light" versions are intended to be produced which will be aimed at High School and Undergraduate level students. This work is the primary concern of Commission I.1 Physicochemical Symbols, Terminology, and Units, the only commission in the division.

The Division remains active with its chemical thermodynamics component, in part through its link with the International Association of Chemical Thermodynamics [IACT] which is an Associated Organisation of IUPAC since 2003. The IACT held its biennial meeting, the 19th IUPAC International Conference on Chemical Thermodynamics, in Boulder, Colorado, USA, during August 2006 with symposia covering a variety of topics related to different phases, theoretical and biophysical aspects.

The International Society of Electrochemistry is also an Associated Organization of IUPAC with a direct link to members of the Division Committee, and has had a direct input in areas such as electrochemical terminology and nomenclature and in one of the division projects.

The number of Division Committee Members that are clearly specialists in the area of biophysical chemistry has increased to three in the current biennium, and 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. A recently approved project is in the area of biophysical thermodynamics and the Division is collaborating in examining the possible the interdivisional and interdisciplinary activities within IUPAC in the area of biological chemistry.

Members of the Division Committee are actively collaborating in several symposia in the IUPAC 2007 Congress as co-chairs, namely in the symposia devoted to Chemistry Protecting the Natural Environment, Materials Chemistry and Nanotechnologies, Theoretical Chemistry and Computer Chemistry, Inorganic Chemistry and Biological and Biophysical Chemistry. It is hoped and expected that these symposia in which the Division is actively involved will lead to new ideas for projects in the next biennium.

The Advisory Subcommittee currently consists of 42 international distinguished scientists and engineers, some of whom are drawn from industry and who cover all the areas of physical chemistry and related areas of interest. The members of the subcommittee are all IUPAC Fellows. The role of the subcommittee is to suggest and identify areas that need to be 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 expert referees for IUPAC proposals. The immediate benefit to the Division from the subcommittee is the reduction of the period needed for assessment of project proposals to a period of weeks rather than months.

The division recognises the interdisciplinary nature of its activities and for this reason has representatives on the Committee for Chemistry Education, the Committee for Chemical Industry and the Subcommittee for Green Chemistry. Additionally, a number of projects being carried out are interdivisional which provides a forum for the exchange of ideas in

different areas of chemistry. The division also has representatives on two commissions of IUPAP. The first is on Commission on Statistical Physics to reflect the strong relation between statistical physics and physical and biological chemistry. The second is on Commission on Symbols, Units, Nomenclature, Atomic Masses, and Fundamental Constants (SUNAMCO).

As stated in previous reports from the Division, it is important to realise that the responsibility for leading and guiding the Division and to encourage and support 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 which is reviewed biennially.

II. ACTIVITIES OF DIVISION I WITHIN THE SIX GOALS IN THE IUPAC STRATEGIC PLAN

The activities of Division I in relation to the six long-range goals are as follows:

a. IUPAC will provide leadership as a worldwide scientific organization that objectively addresses global issues involving the chemical sciences.

Scientific leadership is evident through all the Division's projects through the recommendations which are being established and the technical reports which are produced. The databases which have been implemented are unique and serve as a reference point for all colleagues working in this field, being a good example of how IUPAc has taken a leading role.

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 3rd edition of the Green Book, whose influence has been and will continue to be very significant in education, research, industry, and publishing through the world. This activity has involved the Division consistently during the last ten years.

Leadership is also seen through the cooperation with the Committee of Chemical Education, and a joint project has recently been commenced, which deals with innovative ways to present experiments to undergraduates in a way which is applicable in many countries in a harmonised way.

The Division is represented on the Green Chemistry Subcommittee which addresses the important points of sustainable chemistry which is of increasing concern to society as a whole, and not just to the chemical community.

b. IUPAC will facilitate the advancement of research in the chemical sciences through the tools that it provides for international standardization and scientific discussion.

This is a core aim of the Division. The majority of the Division's projects are geared towards international standardization in the proposal of standard nomenclature and terminology and formats and standard methods for presentation of data. All the projects involve extensive scientific discussion and promote the advancement of chemical sciences through recommendations, technical reports or books.

c. IUPAC will assist chemistry-related industry in its contribution to sustainable development, wealth creation, and improvement in the quality of life.

Its projects, particularly in the area of thermodynamics promote connections to chemistry-related industry via workshops and communications among individuals. Several projects involve members of the task force from industry and the Division is represented on COCI.

The Division is also represented on the Green Chemistry Sub-Committee and is actively involved in the organisation of the recently-established series of IUPAC Green and Sustainable Chemistry Conferences.

IUPAC will foster communication among individual chemists and scientific organizations, with special emphasis on the needs of chemists in developing countries.

The members of the Committee and Advisory Sub-Committee are taken from a wide geographical base as well as topic areas with Physical and Biophysical Chemistry seeks to identify and address the needs of the world-wide chemistry community and give all the tools in an equal way which can help them in their research and communication with each other, by providing a common language and common conventions, through the projects which the division has and is carrying out. The division sponsors conferences all over the world, which includes the needs of chemistry and applied chemistry in developing countries.

Additionally, the Division fosters communications with other associations such as the International Association of Chemical Thermodynamics and the International Society of Electrochemistry, both of which are Associated Organizations of IUPAC. The former is directly associated with the IUPAC Conferences on Chemical Thermodynamics.

The division has a representative on the Green Chemistry Subcommittee which is concerned with the important problem of green and sustainable chemistry, and which includes the particular needs of developing countries.

d. IUPAC will utilize its global perspective and network to contribute to the enhancement of chemistry education, the career development of young chemical scientists, and the public appreciation of chemistry.

The Division has always welcomed Young Observers and encourages them to become involved in Division activities. Two of the Division Committee members in the current biennium were recruited in this way. The Division's Advisory Subcommittee seeks to redress any remaining imbalances. Chemical education is a concern in all the projects involving recommendations for terminology and data presentation and in the publishing of books and monographs. Joint projects with the CCE are important for standardising protocols for experimentation. The public appreciation of chemistry is inherent in most of the Division's activities.

e. IUPAC will broaden its national membership base and will seek the maximum feasible diversity in membership of IUPAC bodies in terms of geography, gender, and age.

The Division has actively sought to have a membership in its committee which reflects IUPAC as a global organisation in terms of geography, gender and age. In the last biennium these efforts have borne more fruit than previously and so this has been more successfully achieved. Nevertheless, it remains a difficulty to attract interested younger colleagues, who are often at crucial points in their career, to agree and to be able to devote time to IUPAC activities.

In their totality, the projects of Division I embody all of the six long-range goals of IUPAC. Some projects support certain goals more strongly than other projects depending on the nature of the project

III. PROJECTS WITH UPDATED PROGRESS REPORTS

This section contains the list of all projects underway together with their current brief progress reports. These include the 17 Current Projects, the four projects nearing completion, the five other interdivisional projects and the single project in review at the time of writing this report.

A. CURRENT PROJECTS

1. 1999-037-2-100 - Evaluation of kinetic data for atmospheric chemistry

The objectives of this project are to enhance the accessibility and availability of the evaluated kinetic database, to develop and implement a way to update material on the website to include various linkages and the creation of a mirror website at IUPAC in North Carolina.

By the end of 2006 the data base was migrated to the Website (http://www.iupac-kinetic.ch.cam.ac.uk/) and comprises now more than 900 data sheets including gas phase, photochemical and heterogeneous reactions of atmospheric interest. Two new subcommittee panel members have been taken on board (M. Ammann (PSI, Switzerland), T. Wallington (Ford Motor Co., USA)) in order to compensate for the retirement of R. F. Hampson (NIST, USA). The work of the panel continues along two lines: (a) continuous update of the whole data base whereby all panel members are assigned several tens of reactions, (b) new organisation and representation of the heterogeneous data base that will also include recommendations. Before it was rather a compilation and did not include an evaluation. Four panel members are heavily involved in this effort (R. A. Cox, J. Crowley, M. Ammann and M. J. Rossi). At the same time the mirror site at Research Triangle Park, N.C., is being migrated to a server elsewhere in the US under IUPAC control. This will require the full cooperation of staff in Cambridge (UK) in order to guarantee a flawless transfer of data. The mirror site is visible on the home page of the project. This project seems on track and will continue for some time until the updating routine of all reactions will be in place and successfully handled by new members before the “old guard” begins to retire one-by-one, probably at some time beginning in 2008.

2. 2001-015-1-100 - Standard potentials of radicals*

The aim of this project is to evaluate critically the standard potentials of inorganic and organic radicals in the literature, to recommend values, and to identify reduction potentials for further experimentation. There are two compilations which are now both more than ten years old and in need of updating. The project has compiled new data that has been published since 1989, set up a thermodynamic network and develop in this fashion values for standard potentials that are internally consistent. Data sheets have been prepared for each radical as found in the JANAF tables.

One set of evaluations and eight summary tables have been prepared, including: Inorganic Standard Potentials, Organic Standard Potentials, Gibbs Energies of Formation for Radicals, Inorganic Radical pK_as, Hemicolligation Equilibrium Constants, Inorganic Radical Equilibrium Constants and Radical Henry's Law Constants,. Linked to these tables are individual evaluation sheets which are being prepared.

One particularly challenging task is to obtain a least-squares optimisationfor a thermo-chemical network that links the properties of about 50 radicals, primarily inorganic. Evaluations are complete for most of these radicals and a robust method has been developed for performing the least squares. A confidential web site for the project was created; this web site does not display all of the work conducted by the task group, but it does indicate the general form of the results as they are developing.

The task group met in early June 2007 for the fourth and final time and is now at ~80% completion of the project, with a clear vision of the remaining 20%. One very important benchmark achieved is a consensus on the values of a set of about 10 important reference radical potentials; essential in order to establish final recommendations for the majority of the other recommended potentials. The final set of recommended potentials will consist of several hundred values. A deadline of Dec. 31, 2007 has been set for completion of the first draft of the report. The publication will consist of a few pages of text and several Tables of recommended data. The recommended data will consist of standard potentials involving radicals in aqueous solution, radical pKa's, and related equilibrium constants. This publication will be web-enhanced; the web version will be identical to the printed version, except that each recommendation will have a link to the underlying references, comparisons, and discussion.

3. 2001-028-1-100 - Electrochemical impedance spectroscopy - terminology, nomenclature and data exchange formats

The aim is to summarize, standardize and disseminate the nomenclature of fast developing new fields of application of electrochemical impedance spectroscopy. It seeks to standardize conventions of formats for experimental data exchange and analysis.

The main work has been completed and the paper is now written for two of the three items, namely the aspects of nomenclature and data exchange formats. Terminology is still under discussion. Reductions in the size of the first draft are still being finalised. The first draft of the paper for terminology or definitions aspect resulted in 70 pages, which is currently being reduced to about 20 pages.

4. 2001-030-1-100 - Recommendations on the measurement and analysis of results obtained on biological substances with isothermal titration calorimetry

The aim has been to prepare recommendations for measurement procedures for isothermal titration calorimetry applied to biological substances, the calibration procedures. The recommendations include analysis and reporting of the results in order to facilitate universal comparability of isothermal titration calorimetry (ITC) data from different laboratories.

Measurements have been done for a working standard NAD/NADH binding to a protein, lactate-dehydrogenase for checking the performance of isothermal titration calorimeters. The ‘round-robin’ ITC results from 12 laboratories on the binding of 4-carboxybenzene sulfonamide to carbonic anhydrase were carried out and were evaluated for inclusion in the IUPAC Recommendations.

Draft recommendations have now been prepared including all these aspects and are being finalised.

5. 2002-005-1-100 - Thermodynamics of ionic liquids, ionic liquid mixtures, and the development of standardized systems

The aims of this project are to initiate systematic studies of thermodynamic and thermo-physical properties of Ionic Liquids (IL) based on the needs of industrial chemical processes, to establish a reference system of IL's and (IL + liquid mixtures) with reliable stability and purity and well defined thermodynamic properties, and to define guidelines regarding where research activities and future cooperation should be directed.

Extensive measurements for the standard reference materials have been completed at ten different laboratories around the world, regarding the viscosity, density, thermal conductivity, heat capacity, electrical conductivity, enthalpy of dilution, gas solubility at high pressure, and speed of sound over the temperature range from 238 K to 378 K. The project is going well and should be near completion.

6. 2003-006-1-100 - NMR chemical shifts: updated conventions*

The objectives are to update IUPAC Recommendations 2001: NMR Nomenclature, Nuclear Spin Properties and Conventions for Chemical Shifts [*PAC* 73, 1795 (2001)] by addressing several issues in setting standards for chemical shifts, including temperature variation of the NMR signals of reference compounds, the use of magic-angle spinning for both solutions and solids, solvent effects, and magnetic susceptibility corrections.

Recommendations are given for reporting chemical shifts under most routine experimental conditions and for quantifying effects of temperature and solvent variation, including the use of magnetic susceptibility corrections and of magic-angle spinning (MAS).

This document provides the first IUPAC recommendations for referencing and reporting chemical shifts in solids, based on high-resolution MAS studies. Procedures are given for relating ^{13}C NMR chemical shifts in solids to the scales used for high-resolution studies in the liquid phase. The notation and terminology used for describing chemical shift and shielding tensors in solids is reviewed in some detail, and recommendations are given for best practice.

The provisional recommendations have been in the public review stage until 31 May 2007.

7. 2003-020-2-100 - Ionic liquids database

The aim is to create an open-access, free, on-line, comprehensive database for storage and retrieval of metadata and numerical data for ionic liquids, including their syntheses, structure, properties, and uses.

The collection of data has been assigned among the seven participating laboratories along with the assignment of the development of the WEB outlet for the system and the storage and retrieval system. The database, storage and retrieval systems have been developed at the Thermodynamics Research Centre at NIST. A meeting of the Task Group took place in Beijing, P.R. China in August 2005. The website was officially launched in March 2006 at the American Chemical society Meeting and the database can be accessed at http://ilthermo.boulder.nist.gov/ILThermo/mainmenu.uix. The web site is divided into pure ionic liquids, binary and ternary mixtures and further chemical information.

8. 2003-024-1-100 - Selected free radicals and critical intermediates: thermodynamic properties from theory and experiment

The objective of this project activity is the compilation and critical evaluation of published thermodynamic properties, including the computation of accurate thermo-chemical data for selected free radicals that are of importance in atmospheric and combustion chemistry.

In September 2006 a no-cost extension for this project was requested from IUPAC in order to compensate for the long delay of publication of volume I (*J. Phys. Chem. Ref. Data* **2005**, *34(2)*, 573-656) of the projected three volumes on the thermochemistry of free radicals. This was the reason for the long inactivity of the panel. This no-cost extension until September 30 2007 was granted in November 2006. A meeting of the full panel (except R. Janoschek and Phil Westmoreland) was held in Budapest on 9 and 10 December 2006 in order to resume the activity and regain the initial momentum. Several free radical data sheets were finalized and discussed, however, it seems that several data sheets are still missing for submission. From the Website of the panel (http://atct.anl.gov/IUPAC/assignments.html) it appears that 7 free radical data sheets are ready for submission. The website also displays two additional sections, one for "perennial references" and the other for "project publications" of the group. It should be mentioned that the thermochemistry of several smaller free radicals are being calculated using sophisticated methods in parallel to the compilation of experimental and theoretical literature results. This dual methodology is somewhat delaying the compilation of both experimental and theoretical results for the corresponding free radicals. However, it seems that the original plan of submitting the data sheets of all 32 free radicals of set I will not be on schedule as of September 30 2007 although the data sheets with the most information are in the process of publishing.

9. 2003-036-2-100 - Thermodynamics and non-equilibrium criteria for development and application of supplemented phase diagrams

The aim of the project is to establish rational links between thermodynamic aspects of phase diagrams supplemented by the non equilibrium curve of the glass transition temperature for mixtures of water with vitrifying agents used in the cryo- and dehydro-preservation of natural (foods, seeds, etc.) and synthetic products (pharmaceuticals).

The update and literature classification on supplemental phase diagrams for relevant aqueous systems for food and pharmaceuticals has been completed. The initial critical evaluation of this database to includes the shortcomings of current practice. The information produced so far is available on http://www.iupac.org/publications/cd/phase_diagrams/index.htm.

A technical report will be prepared on how to construct supplemented phase diagrams when there is not enough experimental infomation on a given system. Asecond technical report will dela with the use of such diagrams for different particular cases.
The final review of the drafts will be done at the task group meeting in September 2007.

10. 2004-010-3-100 - Heat capacity of liquids: critical review and recommended values for liquids with data published between 2000 and 2004

The aims are to update and to extend two publications that contained recommended data on liquid heat capacities for almost 2000 mainly organic compounds, "Heat Capacity of

Liquids: Critical Review and Recommended Values", and its "Supplement I" by M. Zábranský, V. Ruzicka, V. Majer (1st work only), and E.S. Domalski published in *Journal of Physical and Chemical Reference Data* in 1996 and 2001. The publications were the product of IUPAC Projects 121/11/87 and 2000-031-1-100.

Updating the databases of experimental data has been completed. New data on calorimetrically measured liquid heat capacities of compounds having their melting temperature below 573 K published in 193 primary literature sources between 1999 and 2006 were entered into computer readable databases.

Compounds were divided into several families (see the previous report). New data for 411 compounds were entered, out of them 202 compounds being new additions, not covered in the previous work. That represents 479 new data sets, each data set consisting of a table of heat capacity and the corresponding temperature. The new additions include data for 3 inorganic compounds and for 50 ionic liquids. Most of the new data cover organic substances (408 compounds, 202 of them new additions).

Data for all compounds from the current databases including the new data are presently being correlated.

At present the timetable is as follows:

1. July 2007: completion of critical assessment of data, correlation
2. December 2007: preparation of manuscript for publication in J.Phys.Chem.Ref.Data
3. Optionally (not part of the 2004-010-3-100 IUPAC project): an amendment and extension of estimation methods for heat capacity of liquids utilizing the updated database of recommended data (Zábranský, M.; Růžička, V. Estimation of the Heat Capacities of Organic Liquids as a Function of Temperature Using Group Additivity. An Amendment. *J. Phys. Chem. Ref. Data* **2004,** *33,* 1071-1081; Kolská, Z.; Kukal, J., Zábranský, M., Růžička, V. Estimation of the Heat Capacity of Organic Liquids as a Function of Temperature by a Three-Level Group Contribution Method, in preparation for *Ind. Eng. Chem. Res.* **2007**).

11. 2004-026-2-100 - Categorizing hydrogen bonding and other intermolecular interactions

The aims are to provide a modern definition of the hydrogen bond by examining comprehensively the various intermolecular interactions in the light of all current experimental and theoretical information. Hydrogen bonded systems both in gaseous and condensed phases in chemical and biological systems will be examined.

The Task Group met in Pisa, on 5-9 September 2005 in the form of a workshop. Eleven out of the fourteen task group members participated in the meeting. All task group members and 10 invited speakers gave talks in the area of hydrogen bonding and molecular interactions. A core-group met in Bangalore between 18 and 22 September 2006. with a one-day discussion including talks by the core-group members and some outside experts. The final report is now being prepoared. A report on the project was published in *Chem. Int*. Mar-Apr 2007, p. 16

12. 2004-035-1-100 - A database of water transitions from experiment and theory

The aims are a critical compilation, experimental determination and validation, and theoretical verification and extension of accurate frequency, energy level, line intensity, line width, and pressure effect spectral parameters of water and all of its major isotopologues.

The present collaborative effort is aimed at devising and constructing a database comprising, eventually, the complete linelist of all major isotopologues of water for studies at all temperatures. To achieve this goal this project will bring together researchers from around the globe who are active in studying the rovibrational spectra of water as well as experts in related data handling. The linelist to be compiled will include theoretical and (where available) experimental values of transition frequencies, intensities, and pressure broadening parameters for all major isotopologues. Emphasis will be on validation, comparisons, and test of the database. To achieve the stated goals of this project requires a concerted effort of experimental and theoretical chemists and physicists, spectroscopists, and computer scientists.

13. 2004-036-1-100 - Establishing recommended data on thermodynamic properties of hydration for selected organic solutes

The objectives are to establish a database of thermodynamic properties of hydration for approximately 200 selected organic solutes at reference conditions of T = 298.15 K and 0.1 MPa and as a function of temperature and pressure up to the near critical region of water, to calculate from the reliable experimental data the values of hydration properties for solutes covering different molecular structures, to use the established database as a standard for testing and deriving new physico-chemical models and methods of molecular simulation to include the development of semi-theoretical prediction schemes for chemical engineering, environmental chemistry and geochemistry.

A first draft paper concerning gaseous solutes has been prepared.

14. 2006-021-2-100 - Liquid intrusion and alternative methods for the characterization of macroporous solids

The aim of this project is to analyse the various liquid intrusion techniques available today to assess the pore-size of materials (with special attention to the pores above 50 nm width), together with other alternatives, in order to provide (i) a critical and comparative appraisal and (ii) an appreciation about the ways which should be favoured and developed to solve the issue described hereafter.

A first step will be made towards satisfactory answers, by listing, examining and evaluating all trials already made in the field. These include the intrusion of safer liquids (other molten metals, water, organics…) and also the extension of the analysis of capillary condensation data up to the macropore range where, for technical reasons it was, until recently, considered inapplicable. In any case, the need of improvement and/or of alternative methods is urgent. By clarifying the situation, this project should help selecting and developing the most promising approaches. The issue concerns most scientists and industrialists working with porous materials (catalysts, pharmaceuticals, building materials, stones of ancient monuments to be restored or protected, adsorbents for chromatography, liquid purification or gas separation …) and it needs an evaluation accepted and used by all persons involved all over the world.

It is planned to present the main conclusions in a conference in May 2008.

15. 2006-023-3-100 - Recommendations for nomenclature and databases for biochemical thermodynamics

The aim is to revise IUPAC Recommendations for Nomenclature and Tables in Biochemical Thermodynamics 1994*. Update these recommendations and increase their usefulness by providing more about computers and databases that have been developed since 1994. Describe the connection between the thermodynamics of enzyme-catalyzed reactions and the kinetics of enzyme-catalyzed reactions that is provided by Haldane relations. These Recommendations will be published as IUPAC-IUBMB Joint Commission on Biochemical Nomenclature (JCBN).

The Sections to be drafted include:
1 Preamble; 2 Introduction; 3 Basic Thermodynamics,4 Thermodynamics of Chemical Reactions; 5 Legendre Transform to Introduce the pH as an Independent Variable in Biochemical Thermodynamics; 6 Equations for the Standard Transformed Formation Properties of a Reactant; 7 Thermodynamics of Biochemical Reactions; 8 Stoichiometry; 9 Standard Apparent Reduction Potentials for Half Reactions of Enzyme-Catalyzed Reactions; 10 Building a Database; 11 Relations Between Biochemical Thermodynamics and Biochemical Kinetics; 12 Nomenclature.
It is expected that the first draft will be completed by the end of 2007.

16. 2006-050-3-100 - Wet surface vibrational spectroscopy experiments*

The aim of this project is to promote the application of wet surface vibrational spectroscopies (ATRIRS, SEIRAS, SERS) to problems in interfacial chemistry by selecting, testing, and disseminating to universities a collection of experiments suitable for undergraduate teaching laboratories and able to be performed with inexpensive equipment.

Undergraduate experiments in interfacial chemistry are presently dominated by measurements of macroscopic quantities such as surface tension and amount adsorbed when increasingly spectroscopic and microscopic data are presented in the corresponding lectures. IUPAC can take a lead in encouraging a more modern molecular approach to interfacial physical chemistry through international collaboration of leading expertise to compile and test a series of appealing experiments which can be readily carried out in undergraduate laboratories with relatively inexpensive equipment.

This project brings together leading physical chemists in the fields of attenuated total reflection infrared spectroscopy (ATRIRS), surface enhanced infrared spectroscopy (SEIRAS), and surface enhanced Raman spectroscopy (SERS), to select practicable experiments which can be carried out in teaching situations throughout the world. Both SERS and SEIRAS employ finely divided metal surfaces while the ATRIRS particle film approach can be applied to any solid. All of the chosen surface spectroscopies are applicable to solid/aqueous interfaces that are of considerable interest in studies of natural and technological systems.

The experiments will be tested and refined in their laboratories of origin, followed by testing in at least two university undergraduate laboratories elsewhere under normal laboratory conditions.

This project has just begun. A meeting of the Task Group is planned for September 2007.

17. 2007-002-1-100 - Guidelines for modulated-temperature differential scanning calorimetry (MTDSC)

Modulated-temperature differential scanning thermal analysis techniques are widely used in many fields. Particularly in pharmaceutical, food and polymer studies where first order transitions, glass transitions and polymorphism are key issues. All sorts of relaxation phenomena as well as coupled thermal and kinetic contributions can advantageously be investigated and selectively studied with such techniques. Typically, calorimetric measurements are subject to systematic errors especially when they depend upon the choice of physical parameters such as amplitude and period of modulation and the temperature scanning rate. Not only the instrument used plays an important role but the sample itself to investigate requires the parameters to be tuned to optimize the response of the instrument in order to eliminate systematic errors and get full unambiguous information. It has to be recognized that whatever the instrument and the associated methodology used the same quantitative information must be obtained on a given sample.

Extension will be made to thermal analysis techniques, where a modulation is superimposed to the temperature ramp, underlying the basic principles and the derived mathematical description of the data treatment. The different methods of measurement and calculation of the main thermodynamic quantities, such as specific heat capacities, first order transitions and glass transitions, will be carefully analyzed. On the different typical aspects associated to the techniques clear description will be made of the operating procedures and methodologies. The project should bring a consistent set of recommendations to be internationally accepted for the use of modulated-temperature calorimetry.

The first meeting of the task group is scheduled for August 2007.

* *Interdivisional project*

B. PROJECTS NEAR COMPLETION OR IN PRESS

1. 110/2/81 - Revision of "Quantities, Units and Symbols in Physical Chemistry" and the Appendices (3rd edition)

The objective is to revise the 2nd edition of "Quantities, Units and Symbols in Physical Chemistry" and the Appendices.

This Commission I.1 project consists of preparation of the third edition planned. The draft version was circulated at the GA held in Brisbane in 2001. After a period of little progress the momentum was regained in 2005. A meeting held in Beijing in 2005 enabled final decisions to be made with respect to public review of the text of the new edition. The public review was completed in March 2006, all suggestions were considered at a Commission meeting in August 2006 and necessary alterations made. The index was prepared and the final text has recently been sent in April 2007 to the Royal Society of Chemistry for printing. Publication is expected by the end of July 2007 before the Torino General Assembly.

2. 120/15/95 - Thermochemistry of chemical reactions: nomenclature, symbols and experimental methods for bond energies

The Technical Report describing this project has been submitted, reviewed and accepted by the ICTNS with recommended change in the organisation of the report to reflect both Recommendations and content of a Technical Report. The revisions are being considered.

3. 150/24/95 - Spectroscopy under extreme conditions of temperature and pressure

The objectives are to obtain international agreement on methods and standards and to prepare documents to guide workers in the field of spectroscopy under extreme conditions. Initially vibrational and electronic spectroscopy will be considered, but the project may be extended to NMR, Mossbauer, and other spectroscopies if the early work reveals interest in these areas. The main issues to be pursued come under the three general headings Instrumentation, Pressure Calibration, and Temperature Calibration. Instrumentation includes the consideration of cell design, the use of membranes with diamond anvil cells, the properties of optical windows under extreme conditions, the design of spectrometers and microscopes, the use of optical fibres for safe access to difficult experimental situations, and the simultaneous generation of high pressure and low temperature in an optical cell. The calibration issues include methods and standards for the calibration of hydrostatic and very non-hydrostatic pressures. Emphasis will be on calibration through the spectroscopic properties, with the intention to make recommendations in the final report of standard substances, inorganic, organic and biological, whose spectroscopic properties can be used for calibration and for establishing the performance of apparatus.

After a period without progress reports, the latest information is that this project will be completed.

4. 2000-026-1-100 - Critical compilation of vapour liquid critical properties

The objective is to review all measurements of vapour-liquid critical properties for pure organic compounds containing **nitrogen**, **halogen**(s), and **sulphur** and **silicon** and to recommend values for critical temperature, critical pressure and critical densities, with uncertainties.

To date, the project has resulted in nine review papers (Parts 1 to 9) published in the *Journal of Chemical and Engineering Data*.

Part 10. Organic Compounds containing Halogen. A draft manuscript on this extensive set of compounds has been sent out for final review, with submission to the Journal of Chemical and Engineering Data planned for next month.

Part 11 on Multifunctional Organic Compounds, and Miscellaneous Compounds for which Data had been published since the earlier Items in this Series.
Work on this is well advanced, with recent assistance from Alan Abramson, who has a very comprehensive collection of critical property data, and who was not previously involved.

The proposed Part 12, on Inorganic Compounds and Elements, has not progressed for some time but steps are being taken to include new members of the task force so that this can move ahead.

C. PROJECTS RECENTLY COMPLETED

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

The widely different data obtained for the viscosity of molten iron and aluminum will be critically reviewed via an interlaboratory comparison and recommended values will be proposed.

The available experimental data for the density and viscosity of liquid aluminum and iron were critically examined with the intention of establishing a density and a viscosity standard. All experimental data were categorized into primary and secondary data according to the quality of measurement specified by a series of criteria. The proposed standard reference correlations for the density of the aluminum and iron are characterized by standard deviations of 0.65 and 0.77% at the 95% confidence level respectively.

The final manuscript was approved by ICTNS in June 2005. The report was published in *J Phys. Chem. Ref. Data,* Vol. 35, No. 1, pp. 285-300, 2006> doi:10.1063/1.2149380

2. 2005-016-1-100 - Developments and applications in solubility*

A book "Developments and applications in solubility" ed. T.M. Letcher was published by the Royal Society of Chemistry in February 2007.

Solubility is one of the most basic and important of thermodynamic properties, and a property which underlies most industrial processes. This book is a collection of 24 chapters involving recent research works, all related to solubility. The objective brings together research from disparate disciplines which have a bearing on solubility. The book highlights the Theory, Techniques, interesting and new Results, Modeling and Simulation, and Industrial Applications related to solubility.

The book has its origins in committee meetings of the International Association of Chemical Thermodynamics. It is a project produced under the auspices of the International Union of Pure and Applied Chemistry (IUPAC). In true IUPAC image, the authors, which represent some of the most important names in their respective fields, come from many countries around the world, including: Australia, Austria, Finland, France, Germany, Ireland, Netherlands, New Zealand, Portugal, Slovenia, South Africa, Switzerland, Poland, United Kingdom and the United States of America.

3. 2005-048-2-100 - Solubility and thermodynamic properties related to environmental issues*

A book "**Thermodynamics, Solubility and Environmental Issues**" ed. T.M. Letcher was published by Elsevier in April 2007.

Environmental problems are becoming an important aspect of our lives as industries grow apace with populations throughout the world. Thermodynamics, Solubility and Environmental Issues highlights some of the problems and shows how chemistry can help to reduce these them. The unifying theme is Solubility – the most basic and important of thermodynamic properties. This informative book looks at the importance and applications of solubility and thermodynamics, in understanding and in reducing chemical pollution in the environment. Written by experts in their respective fields and representing the latest findings in this very important and broad area. A collection of twenty-five

chapters cover a wide range of topics including; mining, polymer manufacture and applications, radioactive wastes, industries in general, agro-chemicals, soil pollution and biology, together with the basic theory and recent developments in the modelling of environmental pollutants.

* Interdivisional project

D. OTHER INTERDIVISIONAL PROJECTS

1. 2001-036-1-300 - Glossary of terms in photocatalysis and radiation catalysis (Division III)

2. 2003-056-2-500 - Standard definitions of terms relating to mass spectrometry (Division V)

3. 2004-005-2-500 - Comparable pH measurements by metrological traceability (Division V)

4. 2004-021-1-300 - Reference methods, standards and applications of photoluminescence (Divisions III and V)

5. 2005-042-1-300 - Chemistry for Biology - an inventory of interdivisional and interdisciplinary activities within IUPAC in the field of biological chemistry (Division III)

E. PROJECTS IN REVIEW

1. 2007-001-02 Evaluated Kinetic Data for Atmospheric Chemistry (supplement to 1999-037-2-100)

2. 2007-015-1 Future energy: Sustainable and clean energy alternatives for our planet*

* Interdivisional project

Other projects in the final stages of preparation for submission are (as of June 2007) :

- A “light” version of the Green Book and translations of the Green Book from English to other languages
- physical chemistry of the actinides

IV PUBLICATIONS AND PROJECT LIST

IV.1 LIST OF PUBLICATIONS SINCE 2000

A.1 REPORTS

Evaluated kinetic and photochemical data for atmospheric chemistry: Volume III - gas phase reactions of inorganic halogens
Atmos. Chem. Phys. **7**, 981-1191 (2007**)**

Evaluated kinetic and photochemical data for atmospheric chemistry: Volume II - gas phase reactions of organic species
Atmos. Chem. Phys. **6**, 3625-4055 (2006**)**

Standards, calibration, and guidelines in microcalorimetry. Part 2. Calibration standards for differential scanning calorimetry
(IUPAC Technical Report)
Pure Appl. Chem. **78**(7), 1455-1476 (2006)

Vapor-Liquid Critical Properties of Elements and Compounds. 9. Organic Compounds Containing Nitrogen
J. Chem. Eng. Data; **51**(2), 305-314 (2006)

Reference data for the density and viscosity of liquid aluminum and liquid iron
J. Phys. Chem. Ref. Data, **35**(1), 285-300 (2006)

Atomic force microscopy and direct surface force measurements
(IUPAC Technical Report)
Pure Appl. Chem. **77**(12), 2149-2170 (2005)

Evaluated kinetic data for combustion modeling: supplement II
J. Phys. Chem. Ref. Data, **34**(3), 757-1397 (2005)

Measurement and interpretation of electrokinetic phenomena
(IUPAC Technical Report)
Pure Appl. Chem. **77**(10), 1753-1805 (2005)

IUPAC Critical Evaluation of Thermochemical Properties of Selected Radicals: Part I.
J. Phys. Chem. Ref. Data **34**, 573-656 (2005)

Practical guide to measurement and interpretation of magnetic properties
(IUPAC Technical Report)
Pure Appl. Chem. **77**(2), 497-511 (2005)

Electrochemistry at the interface between two immiscible electrolyte solutions
(IUPAC Technical Report)
Pure Appl. Chem. **76**(12), 2147-2180 (2004)

Evaluated kinetic and photochemical data for atmospheric chemistry: Volume I - gas phase reactions of O-x, HOx, NOx and SOx species
Atmos. Chem. Phys. **4**, 1461-1738 (2004**)**

Quantities, terminology, and symbols in photothermal and related spectroscopies
(IUPAC Recommendations 2004)
Pure Appl. Chem. **76**(6), 1083-1118 (2004)

Measurement of pH. Definition, standards, and procedures
(IUPAC Recommendations 2002) (V, I)
Pure Appl. Chem. **74**(11), 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
J. Phys. Chem. Ref. Data, **30**(5), 1199-1689 (2001)

NMR nomenclature. Nuclear spin properties and conventions for chemical shifts (I.5)
Pure Appl. Chem. **73**(11), 1795-1818 (2001)

Standards in isothermal microcalorimetry (I.2)
Pure Appl. Chem. **73**(10), 1625-1639 (2001)

Quantum chemical B3LYP/cc-pvqz computation of ground-state structures and properties of small molecules with atoms of *Z* £ 18 (hydrogen to argon) (I.5)
Pure Appl. Chem. **73**(9), 1521-1553 (2001)

Use of Legendre transforms in chemical thermodynamics (I.2)
Pure Appl. Chem. **73**(8), 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), 381-394 (2001)

Vapor-Liquid Critical Properties of Elements and Compounds: Part 8. Organic Sulfur, Silicon and Tin Compounds (I.2)
J. of Chem. and Eng. Data **46**, 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), 1449-1452 (2000)

Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry. Supplement VIII (Halogen Species) (I.4)
J. Phys. Chem. Ref. Data **29**, 167-266 (2000)

A.2 BOOKS

Developments and applications in solubility, ed. T.M. Letcher
Royal Society of Chemistry, February 2007.
(from 2005-016-1-100 - Developments and applications in solubility*

Thermodynamics, solubility and environmental issues, ed. T.M. Letcher
Elsevier, April 2007.
(from 2005-048-2-100 - Solubility and thermodynamic properties related to environmental issues*

Revision of "Quantities, Units and Symbols in Physical Chemistry" and the Appendices (3rd edition)
(continuation of 110/2/81). The 3rd Edition will be published by the Royal Society of Chemistry /IUPAC in July 2007.

A.3 DATABASES

Kinetics database on http://www.iupac-kinetic.ch.cam.ac.uk/**. More than** 9000 dfata sheets have been published.

Standard potentials of radicals. Data are availbale on
http://atct.anl.gov/IUPAC/assignments.html and are being increased in size.

Ionic liquids datbase. Thers data are availbale on
http://ilthermo.boulder.nist.gov/ILThermo/mainmenu.uix

Supplemental phase diagrams
http://www.iupac.org/publications/cd/phase_diagrams/index.htm

A.4 CHEMISTRY INTERNATIONAL 2006-7

"The project place"

Categorizing hydrogen bondiong and other intermolecular interactions
Chem. Int., March-April 2007, 16.

"Making an Impact"

Evaluated kinetic data for combustion modelling
Chem. Int., Jan-Feb 2006, 30.

Atomic force microscopy and direct surface force measurements
Chem. Int., March-April 2006, 32-33.

Reference data for the density and viscosity of liquid aluminium and liquid iron
Chem. Int., May-June 2006, 20-21.

“Tools of the trade”

Using InChI, J.G. Frey
Chem. Int., Nov-Dec. 2006, 14-15.

Evaluated kinetic and photochemical data for atmospheric chemistry, M.J. Rossi
Chem. Int., Jan-Feb. 2007, 15-16.

“Conference call”

Chemical thermodynamics, J.H. Dymond, M. Frenkel
Chem. Int., March-April 2007, 24-26.

B. LIST OF PROJECTS

B.1 CURRENT PROJECTS

1. 1999-037-2-100 - **Evaluation of kinetic data for atmospheric chemistry**
2. 2001-015-1-100 - **Standard potentials of radicals***
3. 2001-028-1-100 - **Electrochemical impedance spectroscopy - terminology, nomenclature and data exchange formats**
4. 2001-030-1-100 - **Recommendations on the measurement and analysis of results obtained on biological substances with isothermal titration calorimetry**
5. 2002-005-1-100 - **Thermodynamics of ionic liquids, ionic liquid mixtures, and the development of standardized systems**
6. 2003-006-1-100 - **NMR chemical shifts: updated conventions***
7. 2003-020-2-100 - **Ionic liquids database**
8. 2003-024-1-100 - **Selected free radicals and critical intermediates: thermodynamic properties from theory and experiment**
9. 2003-036-2-100 - **Thermodynamics and non-equilibrium criteria for development and application of supplemented phase diagrams**
10. 2004-010-3-100 - **Heat capacity of liquids: critical review and recommended values for liquids with data published between 2000 and 2004**
11. 2004-026-2-100 - **Categorizing hydrogen bonding and other intermolecular interactions**
12. 2004-035-1-100 - **A database of water transitions from experiment and theory**
13. 2004-036-1-100 - **Establishing recommended data on thermodynamic properties of hydration for selected organic solutes**
14. 2006-021-2-100 - **Liquid intrusion and alternative methods for the characterization of macroporous solids**
15. 2006-023-3-100 - **Recommendations for nomenclature and databases for biochemical thermodynamics**
16. 2006-050-3-100 - **Wet surface vibrational spectroscopy experiments***
17. 2007-002-1-100 - **Guidelines for modulated-temperature differential scanning calorimetry (MTDSC)**

* Interdivisional project

B.2 PROJECTS NEAR COMPLETION OR IN PRESS

1. 110/2/81 - **Revision of "Quantities, Units and Symbols in Physical Chemistry" and the Appendices (3rd edition)**

2. 120/15/95 - **Thermochemistry of chemical reactions: nomenclature, symbols and experimental methods for bond energies**

3. 150/24/95 - **Spectroscopy under extreme conditions of temperature and pressure**

4. 2000-026-1-100 - **Critical compilation of vapour liquid critical properties**

B.3 PROJECTS RECENTLY COMPLETED

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

2. 2005-016-1-100 - **Developments and applications in solubility***

3. 2005-048-2-100 - **Solubility and thermodynamic properties related to environmental issues***

* Interdivisional project

B.4 OTHER INTERDIVISIONAL PROJECTS

1. 2001-036-1-300 - **Glossary of terms in photocatalysis and radiation catalysis** (Division III)

2. 2003-056-2-500 - **Standard definitions of terms relating to mass spectrometry** (Division V)

3. 2004-005-2-500 - **Comparable pH measurements by metrological traceability** (Division V)

4. 2004-021-1-300 - **Reference methods, standards and applications of photoluminescence** (Divisions III and V)

5. 2005-042-1-300 - **Chemistry for Biology - an inventory of interdivisional and interdisciplinary activities within IUPAC in the field of biological chemistry** (Division III)

B.5 PROJECTS IN REVIEW

2007-001-02 **Evaluated Kinetic Data for Atmospheric Chemistry (supplement to 1999-037-2-100)**

2007-015-1 **Future energy: Sustainable and clean energy alternatives for our planet***

* Interdivisional project