IUPAC DIVISION I: PHYSICAL AND BIOPHYSICAL CHEMISTRY

REPORT to COUNCIL and to the IUPAC Secretariat for the biennium 2008-2009

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I. EXECUTIVE SUMMARY AND HIGHLIGHTS

The Physical and Biophysical Chemistry Division (PBCD) has continued its activities in both physical and biophysical chemistry according to the charter of the Division. The composition of the Division Committee is chosen to cover all different areas of physical and biophysical chemistry in order to identify areas to which the division can make new contributions.

For the biennium 2008-09, the Division has 25 projects running, 9 nearing completion or recently completed, and 7 on-going interdivisional with lesser involvement of Division I. This total compares with 26 for the 2006-07 and 28 for the 2004-05 biennium, representing a slight reduction as the Division continues to focus its efforts on fewer but better funded projects. The erosion of the US $ may also explain some of the decrease. 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, whether or not 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 briefly described in articles in Chemistry International. A cumulative list of publications is presented in Section IV of this report.

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

The focal points of the activities of Division I for the biennium 2008-09 are as follows:
(1) **The publication of the third edition of the Green Book** (project no. 110/2/81; http://www.iupac.org/web/ins/110-2-81), resulting from the activities of the Subcommittee on Symbols, Terminology and Units in Physical Chemistry, was published just on time for the GA in Torino (August 2007) and was met with great acclaim with 782 copies sold as of April 2009. This long-term effort has to be understood as a service to the chemistry community at large as the royalties benefitting IUPAC (10% of net revenue from book sales) do not cover the investment in the project by far. Building on this success, Division I supports two follow-on projects: (a) the underwriting of a **student edition** of the Green Book (project no. 2007-032-1-100; http://www.iupac.org/web/ins/2007-032-1-100), and (b) the **preparation of the translation** of the Green Book into six languages (German, French, Italian, Turkish, Japanese, Portuguese) (project no. 2008-007-3-100; http://www.iupac.org/web/ins/2008-007-3-100). IUPAC does not support the translation per se, only the preparations in order to minimize errors in translation. This guarantees a virtually errorless translation and transcription of the symbols, formulas and units into a foreign language. Other languages into which the Green Book should be translated in high priority would be Spanish, Chinese and Russian. It remains to be seen to what extent the web may be involved in the dissemination of the content of the Green Book, either in its full version or as an abridged version of the forthcoming student edition.

(2) **Creation and Maintenance** of Physical and Biophysical **Data Bases** that are **critically evaluated** are seen as one of the core activities of IUPAC. Much has been said in the past about the difference between a mere compilation (collation) of data and a critically evaluated data base comprising rational recommendations that are discussed and decided upon by a recognized international panel of experts. In the following "Data Base" is understood as being critically evaluated because in our experience it is this kind of data that the user increasingly demands. These activities are seen as central to the activity of Division I, especially in the long term. Five examples may be given: (a) the Atmospheric Chemistry

data base spanning all atmospheric processes except in the liquid phase (cloud and fog chemistry) (original project no. 141/3/89 (http://www.iupac.org/web/ins/141-3-89), follow-on projects no. 1999-037-2-100 (http://www.iupac.org/web/ins/1999-037-2-100) and following, the latest one being 2007-001-2-100 (http://www.iupac.org/web/ins/2007-001-2-100)) performed by the Subcommittee on the Evaluation of Kinetic Data for Atmospheric Chemistry, (b) the H_2O spectroscopic data base regarding line positions and line strengths of all known isotopomers of H_2O (project no. 2004-035-1-100 (http://www.iupac.org/web/ins/2004-035-1-100)), (c) the Comparison of Experimental and Theoretical Heats of Formation of Free Radicals and Reactive Transients (project no. 140/9/97 (http://www.iupac.org/web/ins/140-9-97), 2000-013-1-100 (http://www.iupac.org/web/ins/2000-013-1-100)), (d) Evaluated Kinetic Data for Combustion Modeling (project no. 140/6/93 (http://www.iupac.org/web/ins/140-6-93), 2005-036-1-100 (http://www.iupac.org/web/ins/2005-036-1-100)) and the Standard Potentials of free radicals in solution (project No. 2001-015-1-100 (http://www.iupac.org/web/ins/2001-015-1-100)). In terms of practical needs by the chemistry community several data bases might be of interest some time in the near future, among them a data base on the kinetics of atmospheric processes in aqueous solution for the description of cloud and fog processing chemistry. One should not forget that this type of data base is at the origin of complex climate simulation schemes performed within the framework of the renowned Fourth Assessment Report (FAR 2007) of IPCC: http://www.ipcc.ch/ipccreports/ar4-syr.htm), a project that was awarded the 2007 Nobel peace prize (R. Pachauri).

Other suggestions of future creations of critically evaluated data bases might be the processing kinetics data base for electronic materials, both in the gas as well as in the condensed phase, and planetary and/or interstellar chemistry including kinetics and thermodynamics (at low to ultralow temperatures) in order to support our understanding of extraterrestrial planetary phenomena. This kinetic and thermodynamic information will enhance our understanding of potential run-away phenomena in the context of global change that may threaten the survival of our planet in the future. In conjunction with the **management** of such **data bases** the question regarding the servicing of the data (updating the information, adding new processes, expanding the scope in response to new questions and new research) may be posed. IUPAC would be well advised to find a definitive answer within a few years in order to preserve the heritage for generations of chemists to come and to protect the considerable effort and investment made by IUPAC. New ways to operate must be found for new ways to deal with easily accessible albeit prolific information assembled in data bases.

(3) For the foreseeable future Division I is motivated to tackle **Energy-related Questions** and in fact, already has made inroads into this technologically important field. Several aspects are within reach and expertise of Division I: (a) Energy Storage; (b) Hydrogen Economy (see for example 2008-006-3-100 (http://www.iupac.org/web/ins/2008-006-3-100)); (c) Materials Chemistry and Corrosion Issues; (d) Alternative fuels and biofuels, some of the topics perhaps in collaboration with Div III (Organic/Green chemistry) and VI (Environment). These subjects touch upon technologies requiring a chemistry background to answer relevant questions on the molecular level. Typical Div I subjects such as electrochemistry, surface chemistry, kinetics, thermodynamics and solid state chemistry are all part of the solution to technological problems in the energy-related field. Monographs authored by multiple experts offering detailed views into a field and describing the state-of-the-art provide a rapid and

efficient entry to complex fields of expertise. Examples are the IUPAC (book) projects coordinated by T. Letcher in the field of energy (project no. 2007-015-2-100 (http://www.iupac.org/web/ins/2007-015-2-100): Future Energy: Improved, sustainable and clean options for our planet) and climate change (project no. 2007-050-2-600: Climate and global change: observed impacts on planet earth (http://www.iupac.org/web/ins/2007-050-2-600)). **Materials chemistry** is an emerging and important area in Material Sciences (and has remained so for some time) but has so far not found a "home" within IUPAC. Division I is prepared to host and nurture this "orphan" for the time being (see below).

(4) Division I is acutely aware that many **solutions to complex problems** are only accessible through an **interdisciplinary or transdisciplinary approach**. Albeit supported by IUPAC in a significant way through its Project Committee (PC) it turns out that such multidisciplinary projects have several hurdles to overcome in practice, not the least of which is the way such a project is perceived by the various concerned divisions of IUPAC. Often, funding levels agreed by the concerned divisions are seriously deficient, time lines are unilaterally extended, if not ignored, and priorities and due diligence are left wanting. It is suggested to commit a substantial amount of financial power to **problem-oriented questions** that often evidently transcend the classification into traditional disciplines. In addition to a vertically oriented structure in terms of Divisions following the traditional classification, a horizontal (orthogonal) layer of management dealing with cross-disciplinary questions could co-exist naturally without interference by the classically organized divisions. This would introduce a 2-D "maze" of management structures optimally suited to respond to the challenge of cross-disciplinarity. Global change is a vivid example of a combination of problems, addressing both "classical" disciplines as well as interdisciplinary approaches. It is clear that no single ("disciplinary") approach affords a satisfactory solution, only concerted action in all compartments may lead the way to a viable solution. Although this has been known for some time now, the science structure only slowly and hesitantly resolves itself to address these overarching issues.

Division I has therefore taken the decision to join two interdivisional activities in the making, Green Chemistry inititated by the president of Div III (P. Tundo) and Materials Chemistry initiated by L. Interrante, secretary of Div II. Regarding the first initiative a proposal for the creation of an Interdivisional Committee on Green Chemistry has been submitted to the Executive Committee (EC) via the IUPAC Secretariat by the end of September 2009 after several meetings during the General Assembly 2009 in Glasgow with the participation of P. Tundo (Div III), M.J. Rossi (Div I), A. Fajgelj (Div V) and N. Senesi (Div VI). As things stand the EC has discussed these ideas and the dissemination of the minutes is imminent. Regarding the second initiative on Materials Chemistry the following members have met at Cornell on October 17 2009 upon invitation of C.K. Ober (Div IV): L. Interrante (Div II), A. West (Div II), M.J. Rossi (Div I), A. Wilson (Div I) and R.G. Jones (Div IV). The plan is to create an interdivisional subcommittee on materials chemistry in the interim with further reaching goals on a longer term in keeping with the importance and the role that this field currently holds. A brief account on this meeting may be found in a future issue of Chemistry International (http://www.iupac.org/publications/ci/tocs/ci.html).

(5) **Strengthening of industrial participation** in problem-solving where technology matters. To the extent that chemistry will be part of the solution of a complex technological problem, for example energy-related problems in future mobility in a sustainable world, it is proposed

to actively seek the involvement of the corresponding industry. In some cases it may be an industry other than chemical depending on the problem. It seems clear that industry participation in projects will be different from the open structures in academia as far as keeping key information confidential. However, it may well turn out to be a win-win situation for the industry/academia collaboration: on the one hand, industry has an international partner with an independent opinion or approach, on the other hand IUPAC becomes involved hands-on in a practical realization of theoretical concepts.

The Division remains involved with its chemical thermodynamics component, in part through its link with the International Association of Chemical Thermodynamics [IACT; http://iactweb.org/] which is an Associated Organisation of IUPAC since 2003. The IACT held its biennial meeting, the 20th IUPAC International Conference on Chemical Thermodynamics, in Warsaw during August 2008 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 in one of the division projects.

After the name change from Physical Chemistry Division to Physical and Biophysical Chemistry Division in December 2001 a lot of effort was spent to include biophysical aspects in Div I activities. Seven years in hindsight led to the view that these **biophysical aspects are less well represented than hoped for**, a fact that also is reflected in the low number of biophysically inspired IUPAC projects that Division I previously supported or currently supports. Although some progress was made in the last (2006-2007) and current biennium (2008-2009) in this regard, there still remains a lot to be done in order to fully justify the name of the Division.

The Advisory Subcommittee currently consists of 48 distinguished scientists and engineers, some of whom are drawn from industry and who cover all areas of physical chemistry and related areas of interest. The members of the subcommittee are all IUPAC Fellows. The role of the Advisory 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 lies in the rapid response for assessment of project proposals spanning the range of a few weeks rather than months.

The division 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 (http://www.iupap.org/commissions/c3/members.html). The second is on Commission on Symbols, Units, Nomenclature, Atomic Masses, and Fundamental Constants (SUNAMCO). This representation should be maintained in the near future in order to keep the communication channels open in areas of mutual concern.

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 its growing activities lies on the shoulders of a relatively few individuals, who also have heavy responsibilities in their professional environment. They essentially 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, the membership of which is reviewed biannually.

There are three concerns that have been brought to the attention of the IUPAC Bureau by the Division president on the occasion of one of its recent meetings (Bratislava, April 2009) and which will briefly be mentioned here:
(a) The maintenance of Data Bases. The last updates should not be older than six months. This necessitates technical updating on a semi-regular basis.
(b) The choice of the proper scientific journal for the publication of Technical Reports and reporting of scientific results obtained in the course of an IUPAC project. In special cases the use of a journal other than Pure and Applied Chemistry may be justified.
(c) The sharing of reviewing authority for papers to be published between ICTNS and the corresponding division.

Among the many applications received Div I actively supported the application for Financial Support (AIS) of the Second Regional Symposium on Electrochemistry: South East Europe, 6-10 June 2010, Belgrade, Serbia, submitted by V.B. Miskoviç-Stankoviç. This Symposium taking place in a scientifically emerging region is commended in particular for the scope of its presentations and the gender balance of its invited speakers. The conveners will be able to support a number of young participants from this region to enable their attendance.

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 critically evaluated databases which have been created and are being maintained so far by the original task group members are unique and serve as a resource for all colleagues working in this field, being a good example of how IUPAC has taken a leading role. Citing just two examples it is the atmospheric chemistry data base (project 1999-037-2-100 (http://www.iupac.org/web/ins/1999-037-2-100)) and the water vapour spectroscopy data base (project 2004-035-1-100 (http://www.iupac.org/web/ins/2004-035-1-100)) that serve as a resource for the regularly updated global climate predictions performed by the IPCC (Fourth Assessment Report of the Intergovernmental Panel on Climate Change under the auspices of the UN: http://www.ipcc.ch/ipccreports/ar4-syr.htm). Additional examples are provided by combustion chemistry and reactive transients such as free radicals.

The Commission on Physicochemical Symbols, Terminology, and Units of Division I continues to exert a strong role through the publication of the 3rd edition of the Green Book in August 2007 which has been well received. Its influence will undoubtedly continue to be very significant in education, research, industry, and publishing throughout the world. This activity has involved the Division consistently during the last ten years, and currently there

are significant follow-on projects underway such as a Green Book student edition, web-version and various translation projects that need intellectual support by the Committee.

Leadership is also seen through the cooperation with the Committee of Chemical Education, and a joint project (project 2006-050-3-100 (http://www.iupac.org/web/ins/2006-050-3-100)) 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 and needing only modest resources.

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 one of the core activities of the Division. The majority of the Division's projects are geared towards international standardization in terms of standard nomenclature, 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. In some cases regularly updated websites have been created in addition to hard copy documentation. The example of the atmospheric chemistry data base (IUPAC Subcommittee for Gas Kinetic Data Evaluation) may be cited (http://www.iupac-kinetic.ch.cam.ac.uk/).

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 was actively involved in the organisation of the recently-established series of IUPAC Green and Sustainable Chemistry Conferences.

d. 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 Division Committee and Advisory Sub-Committee of Division I are taken from a broad geographical base as well as topical areas within Physical and Biophysical Chemistry and seek to identify and address the needs of the world-wide chemistry community. The members strive to hand out all the tools in a fair and 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 biannual 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.

e. 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. Several of the Division Committee members in the current and last biennia were recruited in this way, and we are looking forward to welcome additional Young Observers for this coming GA. The Division's Advisory Subcommittee seeks to redress any remaining imbalances. Chemical education is a concern in all the projects involving recommendations for terminology, 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 and will certainly get a boost during the coming biennium with the preparations for the International Year of Chemistry in 2011.

f. 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 current and last biennium these efforts have borne more fruit than previously and so this has been more successfully achieved. Twenty one countries are represented as TM's AM's and NR's of Division I. 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 BRIEF PROGRESS REPORTS

In contrast to the more general goals of IUPAC as a whole (see Section II) the specific objectives of the Physical and Biophysical Chemistry Division, as stated on the Division web page (http://www.iupac.org/web/ins/100), 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.

This section contains the list of all on-going projects together with their current brief progress reports. These include the current Projects, the projects completed during the current biennium and/or the ones nearing completion, the other interdivisional projects and the single project in review at the time of the writing of this report. It is strongly recommended to consult the corresponding website of the Division for more detailed information (http://www.iupac.org/indexes/Projects/bodies/100).

NOTA BENE: The projects with an asterisk * in their titles are interdivisional.

A. CURRENT PROJECTS

1999-037-2-100 – (Cox) 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 and maintenance of a mirror website at IUPAC in North Carolina at the request of the IUPAC Secretariat. 2009 is the tenth anniversary of providing the atmospheric chemistry community with evaluated data, a fact pointed out on the website (http://www.iupac-kinetic.ch.cam.ac.uk/).

By the end of 2006 the data base migrated to the Website (http://www.iupac-kinetic.ch.cam.ac.uk/) and comprises now more than 1000 data sheets including gas phase, photochemical and heterogeneous reactions of atmospheric interest. An additional Subcommittee member (Wahid Mellouki, Orléans) joined the group before a retirement as of 2009 (R. Atkinson) and the imminent retirement of several colleagues in the near future. Tim Wallington (Ford Research, Dearborn, USA) took over the chairmanship from R.A. Cox (Cambridge, UK). He was thanked for his guidance and leadership of the Subcommittee since taking over from Alistair Kerr in 1999 and retired as chairman but will stay on as a member of the Subcommittee. Tony Cox led the group in the critical effort of converting the data base from hard copy to an electronic support that is accessible on the web. He commandeered a project that may serve as a flagship project, certainly for Division I if not for IUPAC as a whole. 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. Prior to this the heterogeneous part was a compilation rather than an evaluation. Four panel members are heavily involved in this effort (R. A. Cox, J. Crowley, M. Ammann and M. J. Rossi). The fate of the mirror site in

North Carolina is uncertain at this time after having been in operation for several years. It is currently not accessible from the project home page.

The full panel met in January 2009 in Cambridge in order to discuss ordinary updates of existing data sheets, additional data sheets on heterogeneous reactions as well as a hecatomb of new data sheets in relation to gas phase oxidation of organic and biogenic hydrocarbons. This project seems on track as the migration of the data sheets to the web is terminated and a final report including a list of publications has been submitted (http://www.iupac.org/projects/1999/1999-037-2-100_final-report_071218.pdf). Dr. Glenn Carver of the Center for Atmospheric Science in Cambridge/UK will remain available to offer technical help for the migration of the remaining data sheets as they become available. It is important to make the distinction between the migration of the data base proper (see above project and its one-time extension) and the continuing projects of the same group that enable the completion of the data base in view of on-going research in this area (project 2007-001-2-100 (http://www.iupac.org/web/ins/2007-001-2-100)). This flag-ship project experiences on average 400 visits of its website per week, which is a respectable success that coincides with its ten-year anniversary of providing atmospheric chemistry data on the web. A list of publications resulting from this project reaching further back is also available (http://old.iupac.org/divisions/I/I.4/141_publications.html).

2001-015-1-100 – (Stanbury) Standard potentials of free radicals*

The aim of this project is to critically evaluate the standard potentials of inorganic and organic radicals in the literature, to recommend values, and to identify reduction potentials for further experimental investigation. 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 have 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_a's, 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 optimisation for a thermo-chemical network that links the properties of about 50 radicals, primarily inorganic, in a manner that recalls the Active Thermochemical Tables (ATcT) of Ruscic and coworkers. A no-cost extension to June 30 2009 has been requested and granted.

2001-028-1-100 – (Stoynov) 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 the terminology or definitions aspect resulted in 70 pages, which is currently being reduced to about 20 pages.

2003-006-1-100 – (Harris) 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.

This project has been completed and the IUPAC Recommendations have been published in PAC (***Pure Appl. Chem*. 80(1), 59-84, 2008**). These Recommendations have been reprinted in several places in the scientific literature (see project website http://www.iupac.org/web/ins/2003-006-1-100). Several publications resulting from project work have appeared in the recent literature whose references may be found on the same website.

2003-024-1-100 – (Rusciç) 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 thermochemical 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 no-cost extension until September 30 2007 was granted in November 2006. The published article has been cited more than 110 times at the date of this writing and clearly demonstrates a need for critically evaluated thermochemistry of reactive transients. A meeting of the full panel (except R. Janoschek and Phil Westmoreland) was held in Budapest on December 9 to 10 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 publication. From the website of the panel (http://atct.anl.gov/IUPAC/assignments.html) that was accessible until a few months ago it appears that 7 free radical data sheets are ready for publication. 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 December 2009. Therefore, closure of this project has been requested with the option of submitting a new proposal under new leadership.

2003-036-2-100 – (Corti) 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 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 has been prepared on how to construct supplemented phase diagrams when there is not enough experimental information on a given system and has been submitted to publication in PAC. A second technical report will deal with the use of such diagrams for different particular cases. The final review of the drafts were supposedly performed at the task group meeting in September 2007. A no-cost extension to April 30 2009 has been granted.

2004-010-3-100 – (Ruzicka) 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 publication 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 121/10/87 (http://www.iupac.org/web/ins/121-10-87) and 2000-031-1-100 (http://www.iupac.org/web/ins/2000-031-1-100).

Updating the database 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 a computer readable database.

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).

By November 2007 the critical assessment of data as well as the correlation has been performed. By the end of March 2008 a manuscript has been submitted to *J. Phys. Chem. Ref. Data* for publication. In addition, an extension of the estimation method for heat capacity of liquids as a function of temperature utilizing the updated database of recommended data (Kolská, Z.; Kukal, J., Zábranský, M., Ružicka, V. Estimation of the Heat Capacity of Organic Liquids as a Function of Temperature by a Three-Level Group Contribution Method) has been submitted for publication to *Ind. Eng. Chem. Res*. This project is considered terminated.

2004-026-2-100 – (Arunan) 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 to 22 September 2006 with a one-day discussion including talks by the core-group members and some outside experts. The presentations are available on the web (http://ipc.iisc.ernet.in/~arunan/iupac). The final report is now being prepared. However, the subject proved to be controversial and the writing of a final report building on scientific consensus does not seem to be as straightforward as it looks owing to scientific disagreement among the task group members. A no-cost extension to December 31 2007 was granted. A report on the project was published in *Chem. Int*. Mar-Apr 2007, p. 16

2004-035-1-100 – (Tennyson) 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 isotopologs.

The present collaborative effort is aimed at devising and constructing a database comprising, eventually, the complete linelist of all major isotopologs of water for studies at all temperatures. To achieve the goal of 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 isotopologs. Emphasis will be on validation, comparison, 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. The first paper on $H_2{}^{17}O$ and $H_2{}^{18}O$ was recently accepted by the Journal of Quantitative Spectroscopy and Radiative Transfer (10.1016/j.jqsrt.2009.02.014). Apparently, two further publications are well underway, and a fourth paper is planned until the end of 2009 after which the task group will be terminated after a final meeting towards the end of the year.

2004-036-1-100 – (Sedlbauer) 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.

2006-021-2-100 – (Rouquerol) 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 the introduction of alternative methods are 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. From the financial records to date it seems that most of the action is yet to come.

2006-023-3-100 – (Alberty) 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.
The first draft has been met with critical acclaim during 2008 such that more work is almost certainly going to be needed. A no-cost extension until December 1 2008 was granted.

2006-050-3-100 – (McQuillan) 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 using 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 using 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. The task group stated in 2009 that progress has been slower than expected. The task group leader envisaged a one year no-cost extension of the project which has been granted. The task group members met in August 2009 after having met in September 2007.

2007-001-2-100 – (Cox) Evaluated kinetic data for atmospheric chemistry. This is essentially a follow-on to the earlier project and serves to update and expand the existing data base in yearly or semiannual workshops. For details see presentation of project 1999-037-2-100 above. The final report has been received by July 2009 and the project is considered completed.

2007-002-1-100 – (Grolier) 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.

2007-024-2-100 (DeLoos) Guidelines for reporting of phase equilibrium measurements

The objective is to come up with a set of recommendations for potential authors seeking to start phase equilibria measurement and reporting of such data. The main focus of these recommendations will be on the documentation issues. This is a joint project with the International Association on Chemical Thermodynamics (www.iactweb.org).

2007-032-1-100 (Marquardt) Green Book - Abridged Version

The goal of this project is to provide an abridged student version of the 3rd edition of the IUPAC Green Book (Quantities, Units and Symbols in Physical Chemistry) suitable for University teaching, and continuing education in an industrial context. The book will consist of 40-50 pages, which will be made available both as printed material and via the web together with appropriate tutorial examples and exercises.

2007-048-2-100 (Ramasami) Assessment of theoretical methods for the study of reactions involving global warming gas species degradation and byproduct formation

The objectives of this project are (i) To review the quantum mechanical methods which have been used to investigate the reactions involving global warming gas species degradation and byproduct formation, and (ii) To assess the performance of the methods used by comparison with experimental data.

2007-055-2-100 (Yamanouchi) Ultrafast intense laser chemistry

By surveying the current and recent investigations on molecules in an ultrashort intense laser field, we elucidate how important these investigations are for fundamental understanding of light-molecule interaction as well as for controlling chemical and biological reaction processes, and propose future research directions in this newly emerging research field.

2007-059-1-100 (Letcher) Heat capacities of liquids and vapours
The purpose is to produce a single, up-to-date volume on all aspects of heat capacity for liquids and vapours, pure substances and mixtures written by the world's experts in each of about 20 subject areas. The outline of the proposed book may be found on the web (http://www.iupac.org/web/ins/2007-059-1-100).

2008-006-3-100 (Sun) Critical evaluation of thermodynamic properties of hydrogen storage materials: metal organic frameworks and metal or complex hydrides*

The primary purpose of the project is to investigate the thermodynamics of hydrogen production and storage, as a basis for the development of materials with improved hydrogen storage capability. This will be a systematic study of hydrogen adsorption/absorption by divided/confined materials (frameworks, for example Metal Organic Frameworks, MOFs, such as Li-MOFs), and the study of hydrogen production by (thermal) decomposition of Metal Hydrides (MHs, such as La-Mg-Ni/TiCrV-hydrides, MgH_2 ,etc.), and Inorganic Hydrides (Complex Hydrides, such as Li(Na, K, Mg)BH_4, Li-N-H, etc.). The project will consist of 3 major components: a. Establishing a comprehensive bibliography; b. Critical evaluation and compilation of the data; c. Creating an open domain XML-based web archive so that the results will be freely available.

2008-007-3-100 (Marquardt) Preparation for the translation of the *Green Book*

The goal of this project is to pave the way and facilitate the process of using the English original computer source files for the preparation of a structurally identical Green Book document in other languages such as German, French, Italian, Turkish, Japanese or Portuguese. In the long run adherence to the present structure will facilitate generating across-the-languages dictionaries that are virtually produced error-free owing to minimal handling of the content.

2008-014-1-100 (Sengers) Experimental Thermodynamics Vol. VIII. Applied Thermodynamics of Fluids

The intent of this volume is to update and reprint Experimental Thermodynamics Volume V, Equations of state for Fluids and Fluid Mixtures (ISBN-10: 0444503846), first published in Oct 2000. This text is out of print and because it was in two volumes with

928 pages it was not always accessible to the intended practitioners within academia, government and industry. The proposed outline of the revised edition may be found at http://www.iupac.org/web/ins/2008-014-1-100.

2008-045-2-100 (Assael) A critical evaluation of the viscosity and density of molten copper and tin.

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. This is a continuation of an earlier effort led by W.A. Wakeham on the properties of molten aluminum and iron (project 2003-005-1-100).

2009-031-1-100 (Wallington) Evaluated kinetic data for atmospheric chemistry

This project will support a meeting scheduled for mid 2010 in order to make progress in the implementation of new kinetic data into the data base and to discuss the modernization of the data base in XML format so as to enable direct transfer of data into large numerical codes simulating the atmosphere and its interaction with the biosphere, lithosphere, hydrosphere and cryosphere.

2009-032-1-100 (Metrangolo) Categorizing halogen bonding and other noncovalent interactions involving halogen atoms.

The term halogen bonding is now in more frequent use. A clear and comprehensive definition across many disciplines is now required and will be of wide benefit in order to avoid confusion. The task requires wide consultation spanning the range from physics to chemistry and molecular biology so that harmonization of views may be achieved in establishing final terminology based on solid observational criteria.

B. PROJECTS NEARING COMPLETION AND/OR RECENTLY COMPLETED

2000-026-1-100 – (Marsh) 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), **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 the immediate future.

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 into the task force so that this can move ahead.

2001-030-1-100 – (Schwarz, Hinz) 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 performed 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.

The final report has been received, published (*Pure Appl. Chem.*, 2008, Vol. 80, No. 9, pp. 2025-2040) and the project is now completed.

2002-005-1-100 – (Marsh) 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 in regards to 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 completed and the findings have been published as Technical Reports in PAC (*Pure Appl. Chem.*, 2009, Vol. 81, No. 5, pp. 781-790 (part I) and Vol. 81, No. 5, pp. 791-828 (part 2)). A list of scientific publications resulting from this project may be found on the web (http://www.iupac.org/projects/2002/2002-005-1-100-publi070702.pdf).

2003-020-2-100 – (Seddon) 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. However, the data base has not been edited since 7/23/2006 which is some reason for concern regarding a field that is expanding at a fast pace. The project has been completed with the submission of the final report at the beginning of 2008.

2003-005-1-100 – (Wakeham) 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. An extension project has been submitted and recently funded (2008-045-2-100 (Assael)).

2005-016-1-100 – (Letcher) Developments and applications in solubility*

A book “Developments and applications in solubility”, T.M. Letcher (ed.) 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.

2005-048-2-100 – (Letcher) Solubility and thermodynamic properties related to environmental issues*

A book "Thermodynamics, Solubility and Environmental Issues", T.M. Letcher (ed.) 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.

2007-015-2-100 (Letcher) Future Energy: Improved, sustainable and clean options for our planet.

The objective is to first consider the reasons for developing alternate forms of energy and to then detail all the possible forms available to us. Each chapter will be written by an engineer or scientist, working in the field. Much of the argument and details of the forms, depend on environmental and chemical issues. The project is now completed and the book titled "Future Energy - Improved, Sustainable and Clean Options for our Planet" has been published by Elsevier in 2008 [ISBN 978-0-08-054808-1]. The outline of the book may be found at http://www.iupac.org/web/ins/2007-015-2-100.

C. OTHER INTERDIVISIONAL PROJECTS (with lesser involvement of Division I)

2001-036-1-300 – (Parmon, Serpone) Glossary of terms in photocatalysis and radiation catalysis
(Division III)

2003-056-2-500 – (I. Murray, K.K. Murray) Standard definitions of terms relating to mass spectrometry
(Division V)

2004-005-2-500 – (Camões) Comparable pH measurements by metrological traceability
(Division V)

2004-021-1-300 – (Brauer, San Román) Reference methods, standards and applications of photoluminescence (Divisions III and V)

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

2007-039-1-024 – (Frenkel) Extension of ThermoML - the IUPAC standard for thermodynamic data communications (Division VI)

2007-050-2-600 – (Letcher) (book project), Climate and global change: observed impacts on planet earth (Division VI)

D. PROJECTS IN REVIEW

2008-037-1 – (Griesbeck) Standard Photochemical Processes* (Division III). The author has indicated his willingness to resubmit this industrial photochemistry project in due time after thorough revision.

IV PUBLICATIONS LIST (since 2000)

Sources: project updates, project websites and projects list taken from the Divisional webpage (http://www.iupac.org/web/ins/100). This list is **not** exhaustive.

IV.1 Reports and scientific papers

Evaluated kinetic and photochemical data for atmospheric chemistry: Volume IV – gas phase reactions of organic halogen species
Atmos. Chem. Phys., **8**, 4141–4496 (2008)

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**)**

Evaluated kinetic and photochemical data for atmospheric chemistry: Volume I – gas phase reactions of O_x, HO_x, NO_x and SO_x species
Atmos. Chem. Phys., **4**, 1461–1738 (2004)

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)

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)

Thermochemical Properties of the Hydroxy-formyl Radical HO CO, and the Formyloxy Radical, HC(O)O, and their Role in the Reaction OH + CO .H + CO_2: Computational G3MP2B3 and CCSD(T)-CBS Studies
J. Mol. Struct. TheoChem **713**, 227 (2005)

Ab Initio Determination of the Heat of Formation of Ketenyl (HCCO) and Ethynyl (CCH) Radicals.
Mol. Phys. **103**, 2159-2168 (2005)

Pulsed Field Ionization Photoelectron-photoion Coincidence Study of the Process N_2 + hν ➔N^+ + N + e^- : Bond Dissociation Energies of N_2 and N_2^+
J. Chem. Phys. **123**, 074330/1-7 (2005)

Thermochemical Properties of Free Radicals from G3MP2//B3 Calculations, Set-2: Free Radicals with Special Consideration of CH_2=CH-C=CH_2, cyclo-C_5H_5, CH_2OOH, HO-CO and HC(O)O.
Int. J. Chem. Kinet. **36**, 661 (2004)

W3 Theory: Robust Computational Thermochemistry in the kJ/mol Accuracy Range.
J. Chem. Phys. **120**, 4129 (2004)

Benchmark Thermochemistry of the Hydroperoxyl Radical.
J. Phys. Chem. A **108**, 3195 (2004)

Vibrational Spectrum and Thermochemistry of the Formyl (HCO) Radical: A Variational Study by the Coupled Cluster CCSD(T) Method with Complete Basis Set Extrapolation.
J. Phys. Chem. A **108**, 5431 (2004)

Thermodynamic Properties of C_1 and C_2 Bromo Compounds and Radicals: A Relativistic ab Initio Study.
J. Phys. Chem. A **108**, 7752 (2004)

Introduction to Active Thermochemical Tables: Several "Key" Enthalpies of Formation Revisited.
J. Phys. Chem. A **108**, 9979 (2004)

Equilibrium Geometry of the Ethynyl (CCH) Radical.
J. Phys. Chem. A **108**, 3030 (2004)

HEAT: High Accuracy Extrapolated Ab Initio Thermochemistry.
J. Chem. Phys. **121**, 11599 (2004)

Enthalpy of Formation of SH.
J. Phys. Chem. A **107**, 2061 (2003)

Equilibrium Structure and Force Field of NH_2.
Phys. Chem. Chem. Phys. **5**, 3359 (2003)

Structural and Thermochemical Properties of the Hydroxymethyl (CH_2OH) Radical: A High Precision Ab Initio Study.
J. Chem. Phys. **119**, 10105 (2003)

Coupled Cluster CCSD(T) Calculations of Equilibrium Geometries, Anharminic Force Fields, and Thermodynamic Properties of the Formyl (HCO) and Isoformyl (COH) Radical Species.
J. Phys. Chem. A **107**, 2343 (2003)

A Variational Study of Nuclear Dynamics and Structural Flexibility of the CH_2OH Radical.
J. Chem. Phys. **119**, 3098 (2003)

Thermochemical Properties of Free Radicals from G3MP2//B3 Calculations.
Int. J. Chem. Kinet. **34**, 550 (2002)

The Enthalpy of Formation of ^2CH.
Mol. Phys. **100**, 3879 (2002)

Anharmonic Force Field, Structure, and Thermochemistry of CF_2 and CCl_2.
Phys. Chem. Chem. Phys. **4**, 3282 (2002)

Pure Appl. Chem. 2008, Vol. 80, No. 9, pp. 2025-2040 (project 2001-030-1-100 Schwarz/Hinz))

Temperature dependence of the ^{1}H chemical shift of tetramethylsilane in chloroform, methanol, and dimethylsulfoxide

J. Magn. Reson. 176 (2005) 87

Measurement of magnetic susceptibility and calculation of shape factor of NMR samples

J. Magn. Reson. **178** (2006) 237

Standardization of chemical shifts of TMS and solvent signals in NMR solvents

Magn. Reson. Chem. **44** (2006) 606

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(a) *Magn. Reson. Chem*. **46** (2008) 582-598 (together with an editorial letter in *Magn. Reson. Chem*. **46** (2008) 507)
(b) *Solid State NMR* **33** (2008) 41-56
(c) *Encyclopedia of Magnetic Resonance (on-line)*, Editors-in-Chief R. K. Harris & R. E. Wasylishen, DOI 10.1002/9780470034590.emrstm1019

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IV.2 BOOKS

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

Thermodynamics, solubility and environmental issues, ed. T.M. Letcher
Elsevier, April 2007.
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Revision of "Quantities, Units and Symbols in Physical Chemistry" and the Appendices (3rd edition)
(Result of project 110/2/81- Revision of "Quantities, Units and Symbols in Physical Chemistry" and the Appendices (3rd edition). The 3rd Edition has been published by the Royal Society of Chemistry /IUPAC in August 2007 coincident with the GA 2007 in Torino.

IV.3 DATABASES on the Web

Kinetics on atmospheric reactions (homogeneous gas-phase, heterogeneous gas-condensed phase and gas-phase photochemical) database on
http://www.iupac-kinetic.ch.cam.ac.uk/**.**

Ionic liquids datbase. Thermodynamic data are available on
http://ilthermo.boulder.nist.gov/ILThermo/mainmenu.uix/ In the meantime this internet site has become inaccessible (as of December 2009).

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

A database of water transitions from experiment and theory on
10.1016/j.jqsrt.2009.02.014