

DIVISION OF PHYSICAL AND BIOPHYSICAL CHEMISTRY

Progress Report for the IUPAC Bureau Meeting Montreal, Canada, April 2016

Angela K. Wilson
President

March 2016

This report states the aims, the membership, and summarises the activities of Division I since the last report to the IUPAC Council Meeting in Busan, South Korea in August 2015.

Division I Aims

The objectives of the Physical and Biophysical Chemistry Division have not changed since the last report. They are stated on the Division web page.

The main goal of the Physical and Biophysical Chemistry Division is to organize and promote the international collaboration between scientists in physical and biophysical chemistry and related fields. In particular, collaborations are encouraged that address problems and formulate recommendations on nomenclature, symbols, units and terminology, as well as conventions in physical and biophysical chemistry.

To this end, projects are supported that:

- foster the dissemination of the recommendations, the monitoring of their translations and 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 physic-chemical data;
- recognize new developments in physical and biophysical chemistry and their fields of applications;
- 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.

Membership (2016-2017)

The Division thanks the members who have served in Division Leadership during the 2014-2015 biennium, including outgoing President Roberto Marquardt, and outgoing Past President Yamouchi. For the 2016-2017 biennium, the composition of the Division Committee is given below. The Division aims to have a leadership group that is representative of major areas of physical and biophysical chemistry as well as emerging areas in which the Division can make new contributions.

The Subcommittee on Symbols, Terminology and Units listed below is largely responsible for the Green Book and its revisions.

The Division is supported by an Advisory Subcommittee of currently 47 members, whose role is to advise on project proposals and evaluations. It is formed of former Division members and is periodically renewed. It will be reviewed again at the off-year meeting.

The Division Committee periodically corresponds with its members giving notice of annual meetings, distributing news items about divisional activities, and encouraging participation.

The composition of the Committee for the biennium 2016-2017 is the following:

President: A.K. Wilson (USA)

Vice-President: K. Bartik (Belgium)

Secretary: A. Friedler (Israel)

Past President: R. Marquardt (France)

Chair of Subcommittee on Symbols, Terminology and Units: J. Stohner (Switzerland)

Titular Members: A. Császár (Hungary), P. Metrangolo (Italy), J. Stohner (Switzerland), Y.H.

Taufiq-Yap (Malaysia), F. van Veggel (Canada), T. Wallington (USA), B. Weckhuysen (Netherlands)

Associate Members: J.L.B.M. de Faria (Portugal), M. Korenko (Slovakia), T.C. Kurten (Finland), V. Tomišić (Croatia), X. S. Zhao (China),

National Representatives: H.R. Corti (Argentina), L. Gonzalez (Austria), F.P. Malik (Pakistan), C.-C. J. Chen (Taiwan), L.A. Montero-Cabrera (Cuba), S.-J. Jeon (Korea), M. Fall (Senegal)

The composition of the Commission on Physicochemical Symbols, Terminology, and Units is as follows:

Chair: J. Stohner (Switzerland)

Secretary: R. Hinde (USA)

Titular Members: Y. Kuroda (Japan), A. J. McQuillan (New Zealand)

National Representatives: M.Choudhary (Pakistan), J. G. Frey (UK), Y. K. Ha (Korea), A. A.

Milchev (Bulgaria), F. Pavese (Italy), M. Quack (Switzerland), D. Schomburg (Germany), S. Smith (Australia)

Projects

A large part of the activities of the Division is focused upon the identification and support of projects. Below is an overview of several of the newest, ongoing, and completed projects from the Division. These projects were largely reported upon in Busan.

Newest projects

Below are overviews from the most recent projects:

Project No. 2014-010-1-100: Transport Properties (Wakeham), full sponsored by Division I. During the production of Experimental Thermodynamics Volume IX, entitled Transport Properties of Fluids: Advances in Transport Properties (project 2013-003-3-100 mentioned below), it became apparent that Chapter 2.15 of the Green Book requires expansion to include the definitions of a number of different diffusion coefficients as well as to remove ambiguity that has appeared in the publication of articles including Experimental Thermodynamics Vol. III, Measurement of Transport Properties of fluids. An IUPAC Recommendation will be produced defining transport properties and the preferred symbols and SI units for incorporation in a revision of the Green Book. The Recommendation will be provided to the Physical and Biophysical Division, the Committee concerned with physic-chemical Symbols, Terminology and Units and to ICTNS. Interested stakeholders would include physical scientists, biological scientists and engineers.

Project No. 2014-021-2-200: Topology Representation in Crystalline Materials (Öhrströhm), partially funded by Division I. The objectives of this project, which is lead by Division II, are:

- (1) To produce guidelines for terms to use in the topological description of metal-organic frameworks, coordination polymers and other crystalline materials that can be described as network compounds.
- (2) To produce guidelines for the use of topological descriptions in the mentioned areas.
- (3) To ensure permanent and stable access to the database containing topological nets and net descriptors.
- (4) To determine the procedure for depositing new network topologies.
- (5) To elaborate recommendations for including the information about network descriptors and topological properties into

crystallographic databases. This project will be a collaboration with the IUCr and it will resolve outstanding issues identified in project 2009-012-2-200: "Coordination polymers and metal organic frameworks: terminology and nomenclature guidelines" as reported in Pure Appl. Chem., 85, 1715–1724, 2013.

Project No. 2014-028-2-100: Elementary Chemical Kinetics at High Temperatures (Turanyi), full sponsored by Division I. High temperature gas-phase reactions are of significant academic and practical importance in many fields including combustion, pyrolysis and process engineering. The group headed by Prof. Baulch regularly issued reports on the evaluated rate parameters of such reactions. Unfortunately this group stopped its activity. The activity of the new group will include (i) evaluation of the rate parameters of the elementary reactions related to basic fuels and also new fuel species like oxygenates; (ii) assessment of the uncertainty limits of the rate parameters; (iii) dissemination of the results using Web techniques the intended stakeholders of the planned data evaluation work include: (i) experimental and theoretical scientists working in gas phase chemical kinetics; (ii) combustion engineers; (iii) chemical engineers modeling industrial problems; (iv) industrial safety specialists. The results will be published in J. Phys. Chem. Ref. Data

Project No. 2015-006-1-100: Energy Storage (Letcher), partially funded by Division I, the largest portion is sponsored by the University of Kwazulu, South-Africa. The collection of 26 chapters of this book project, written by international experts in their field, presents the latest developments in this fast moving field. Most of the energy storing processes currently being researched or being developed commercially are discussed in this one volume and will give the reader the opportunity of comparing the different processes and making it possible to decide which process is best suited for their situation, be it in a country blessed with abundant sunshine, wind, tides, rivers or mountain reservoirs. The technologies discussed in the book include both grid and off-grid energy storage.

2015-002-2-100 - Valiullin – new project on the diffusion in nanoporous materials

Other Current Projects

Project No. 2012-040-1-100: Reference Correlations for the Thermal Conductivity and Viscosity of Fluids over Extended Range of Conditions (vapor, liquid and supercritical region) (Perkins). The aim of the project is to develop reference correlations for the thermal conductivity and the viscosity of fluids over extended temperature and pressure ranges including vapor, liquid and supercritical region. This project is close to completion.

Project No. 2012-044-1: Basic Terminology of Crystal Engineering (Metrangolo/Resnati). The objectives of this project are (1) to produce guidelines for terminology (glossary of terms) in the area of crystal engineering, (2) to ensure that these guidelines are accepted by a large group of leading researchers in the field, and (3) to have these guidelines implemented or referred to in the instructions to authors of leading crystal engineering journals.

Project No. 2012-051-1-100: International Standard for Viscosity at Temperatures up to 473 K (Goodwin, who was replaced by his colleague Prof. J. Fernandez). There is a need for commercially available certified viscosity reference liquids for which viscosity and density is known over a range of temperatures and pressures. In this project a viscosity standard will be determined experimentally and from statistical analyses of samples collected in different locations in Europe and in the US. The outcome of the project will contribute to improve the quality of communications and data exchange related to viscosity measurements.

Project No. 2013-048-1-100: A critical review of the proposed definitions of fundamental chemical quantities and their impact on chemical communities (Stohner). This project aims primarily at providing a technical report containing a critical review of proposed new definitions of the physical quantity amount of substance, and its unit, mole, as well as of its related unit for the quantity mass. This report should strengthen IUPAC's position in the ongoing discussion about the new definition of

the aforementioned units. It is an interdisciplinary project supported conjointly by Divisions I, II and V, as well as by the Committee on Chemical Education and ICTNS.

Project No. 2013-035-1-100: Evaluated kinetic data for atmospheric chemistry (Wallington).

This project is a continuation of a successful series of projects on kinetic data for atmospheric chemistry, carried out by essentially the same task group. The outcome will be a review of new data published in 2013/2014 and a compilation of recommended data for $\geq C_4$ organic and aromatic compounds of atmospheric interest, important for chemistry-climate models in Earth system analyses for global and regional applications. Work from the previous project received a highlighting science feature article in issue 51 (February 2014) of the International Global Atmospheric Chemistry (IGAC) Newsletter.

Results from recently completed projects

Project No. 2011-022-2-100: High Resolution Spectroscopy Database for Water Isotopologues (Tennyson). The database and explanatory recommendations were published IUPAC Technical Reports in PAC in 2014 (Tennyson *et al.*, Pure and Applied Chemistry 86, issue 1, 71-83; *ibid.* issue 12, 1931-1943). Members of this task group have reported on bad experiences with the publication of articles in PAC with the new Publisher De Gruyter. Because of its importance, this item is given special attention at the end of this report.

Project No. 2012-041-1-100: Future Energy Revisited (Letcher). This is a book publishing project: Volumes Properties: Liquids, Solutions and Vapours, eds. E. Wilhelm and T. M. Letcher, Royal Society of Chemistry, Cambridge, UK, 2014, 22 chapters, ISBN: 978-1-849738996. Publication date: 25 November 2014.

Project No. 2013-003-3-100: Experimental Thermodynamics Volume IX: B, Non-Equilibrium Thermodynamics and Applications (Wakeham). This is a book project, and the book was published by the Royal Society of Chemistry in 2015.

Commission on Physicochemical Symbols, Terminology, and Units

The core activity of the Subcommittee, Commission on Physicochemical Symbols, Terminology, and Units (Commission I.1), is the publication and updating of the book "Quantities, Units and Symbols in Physical Chemistry" (the Green Book). Its 3rd edition was published in 2007 by R. Cohen, T. Cvitas, J.G. Frey, B. Holmström, K. Kuchitsu, R. Marquardt, I. Mills, F. Pavese, M. Quack, J. Stohner, H.L. Strauss, M. Takami, and A.J Thor.

The last printing (third printing) was prepared by the Royal Society of Chemistry (RSC) Publishing in 2011 and is already sold out. For the fourth printing, the Commission gathered at the General Assembly in Busan to complete the preparation of the text for the fourth printing.

The Green Book is being translated into several languages. The Japanese and French translation of the third edition have been published recently. There is a Spanish translation of the second edition. A Turkish and Portuguese translation are in preparation. The Italian translation has been completed.

Strategic Planning for the 2016-2017 Biennium

The off-year meeting will take place on August 26-27, 2016 at Michigan State University in East Lansing, Michigan, USA, just after the National Meeting of the American Chemical Society in Philadelphia. The meeting will begin with a symposium, with Titular Members providing invited talks to familiarize one another with their respective research areas. Though most of the recent Division I meetings have focused upon projects and their status, this meeting will focus upon short- and long-term planning for the biennium, not only in terms of projects, but upon other activities that the Division could pursue. There will also be an evaluation session on existing activities.

IUPAC World Chemistry Congress 2017

The Division is already looking towards the 2017 World Chemistry Congress, and thanks the Brazil organizers for the opportunity to be well engaged in the planning of the Physical Chemistry program for the meeting.

Beginning as an outreach activity for the International Year of Chemistry, the Division has had held a video competition and a cartoon competition for high school and college students. After the first year, this competition has focused upon a cartoon competition. As this activity has been undersubscribed, this activity will be reevaluated, and additional/other outreach opportunities will be considered, with a targeted completion by the 2017 World Chemistry Congress.