



DIVISION OF PHYSICAL AND BIOPHYSICAL CHEMISTRY

Report to the 48th IUPAC Council for the 2014-2015 biennium Busan, 12-13 August, 2015

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I. Highlights of divisional activities in the biennium 2014-2015

The 2014 off year-meeting was held in Kloster Kappel am Albis, Switzerland, between May 31 and June 1, 2014. As in the 2012 off-year meeting, the business part was predeceased by a scientific day, when committee members were given the opportunity to explain their work in short oral presentations. This genuinely scientific part of the meeting has again proven very useful, as it helps to bring members closer one to the other by the mutual discovery of the colleagues' scientific work, thus making the common work for the Union easier to accomplish.

The Division has participated in the project referring to a critical assessment of opinions within and outside the Union about the proposed new definition of the mole, the SI unit of amount of substance, and other units or physical quantities (Project No. 2013-048-1-100, see below).

Four new Division I projects were started. Two new interdivisional projects combining Divisions V, II and I, as well as one project having substantial funding from outside the Union were partially supported by Division I. One conference obtained subventions from Division I.

II. Division I activities

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, herewith contributing to *IUPAC Goal No. 1* and *4*;

establish and stimulate the use of methodologies, standards and reference materials in physical and biophysical chemistry, herewith contributing to *IUPAC Goal No. 2*;

encourage the compilation and documentation of critically evaluated physicochemical data; recognize new developments in physical and biophysical chemistry and their 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, herewith contributing to *IUPAC Goal No. 3*.

With the organization of a world wide student cartoon competition, and the preparation of an abridged student version of one of its flagship document, the Green Book, Division I contributes to the enhancement of chemistry education, the career development of young chemical scientists, and the public appreciation of chemistry (*IUPAC Goal No. 5*).

Both via the careful composition of the Division Committee and the different project task groups running under the auspices of Division I, a maximum feasible diversity in membership in terms of geography, gender, and age is approached (*IUPAC Goal No. 6*).

The composition of the Division Committee given below is designed to cover all major areas of physical and biophysical chemistry and to enable identification of topics in which the Division can make new contributions.

The Subcommittee on Symbols, Terminology and Units listed below is essentially 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.

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 2014-2015 was the following, at the beginning of the biennium:

President: R. Marquardt (France)

Vice-President: A. K. Wilson (USA)

Secretary: A. Friedler (Israel)

Past President: K. Yamanouchi (Japan)

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

Titular Members: K. Bartik (Belgium), A.R. Goodwin (USA,†), A. E. Russell (UK), J. Stohner (Switzerland), Y. H. Taufiq-Yap (Malaysia), F. van Veggel (Canada)

Associate Members: A. Császár (Hungary), V.Yu. Kukushkin (Russia),

A. W. Mombrú Rodriguez (Uruguay), X. S. Zhao (China), K. Bhattacharyya (India), J. L. B. M. de Faria (Portugal)

National Representatives: J. Cejka (Czech Republic), S. Hannongbua (Thailand), M. Koper (Netherlands), J. E. G. Mdoe (Tanzania), V. Tomišić (Croatia), A. bin Hasan Susan (Bangladesh), S.-J. Kim (Korea), E. Klein (Bulgaria), M. Korenko (Slovakia), K. E. Laasonen (Finland); H. Corti (Argentina, as provisional member).

The picture below shows some Committee members with companies during the 2014 off-year meeting in Kappel am Albis, Switzerland. Prof. Andrea Russell was excused. To our greatest sadness, Dr. Anthony Goodwin, who was still with us on this photo, passed away on December 13, 2014. He has not been replaced to date.



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

Chair: J. Stohner (Switzerland)

Secretary: R. Hinde (USA)

Titular Members: A. Goodwin (USA), 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)

A replacement for Dr. Goodwin is pending.

The main points addressed in the 2014 off year meeting were the project progress reports, the discussion of future projects and future strategy of the Division. The topics addressed in the previous report as possible project areas of strategic interest for the future have been incorporated into the program of projects to be privileged by the Division. To be highlighted in particular are topics related data standardization between theory and experiments (see the projects on kinetic data for atmospheric chemistry, 2013-035-1-100, and at high temperatures, 2014-028-2-100, mentioned below) and topics related to material sciences, e.g. the project on crystal energy (2012-044-16100). To be mentioned is also the participation of the Division in project 2014-021-2-200. Other fields outlined at the beginning of the biennium, such as biophysical topics, shale gas fracture, the concept of absorption and emission line intensity, and density functional theory still need to be filled with upcoming projects. Other results ensuing the off-year meeting will be addressed below in the chapter “Specific Information”.

Elections of Titular Committee Members (TM) for the next biennium 2016-2017 were held successfully in June, resulting in four new TM elected, whose election has to be validated by the Council. The nomination commission, chaired by the divisional past-president Prof. Kaoru Yamanouchi, set up an equilibrated list of candidates. However, geographical and in particular gender diversity could not be fully satisfied by the results of the ballot, which is to some extent compensated by the proposed new composition of Division officers for the next biennium: Prof. Angela Wilson will become divisional president, Prof. Kristin Bartik will become vice president; Prof. Assaf Friedler will remain divisional secretary and Prof. Roberto Marquardt will become past-president. These names were suggested and approved at the 2014 off year meeting.

III. Specific information

The following topics have receive particular attention during the discussions of the present biennium:

- (1) Some old projects are still running with no cost extensions granted by the Division. The Division Committee is keeping contact with the respective project chair to encourage completion of their project. As mentioned in the 2014 report to the Bureau, the Division Committee has been continuously expressing concern about the longevity of some of the projects. A number of projects that were not completed have been terminated, and marked as such, while projects that were successfully completed were noted as completed. For projects that were terminated, the Division discourages further awards to the project leader, not only by Division I, but by other IUPAC Divisions as well. Freezes on the funding of projects for which there has been funding have been encouraged. Also, the possibility of limiting the amount of time funds are available for a project has been considered. All these measures will be maintained in the near future.
- (2) Since January 2014 De Gruyter has been the new publishing company of Pure and Applied Chemistry (PAC). Members from one divisional task group issued serious complaints about continuous bad experiences during recent publication processes. Record is made here of one major issue referring to problems of following IUPAC rules about symbols: (cit) “the manuscript was not only delayed by the request to correct the appearance of symbols in a few cases but in many more cases the proofs were simply incorrect and did not follow the rules of scientific writing.” It is a request of this Division that all must be done to ensure the correct reproduction of symbols in printed text that follow strictly the recommendations of the Union.
- (3) On some of the book publishing projects, concern was noted by the Division Committee about the need for IUPAC funds, particularly since royalties are garnered

for commercial projects. IUPAC is encouraged to collect royalties on IUPAC-supported projects, and to put some guidelines in place for accomplishing this.

- (4) The Gold Book, and in particular its online version, is still a world wide used tool to access IUPAC recommendations. It was noted that recommendations published quite some time ago by the Division have not been included in the Gold Book (e.g. the recommendations on the hydrogen or on the halogen bond). The need for a new, "Gold Book Commission" was reiterated. That commission should not only be monitoring carefully updates of the Gold Book, it should also work out a clear concept of how it should look like in the future. People are becoming less aware of the Gold Book and they rather go for Wikipedia. We should make the Gold Book the official definition and have Wikipedia etc. refer to this. It should be the first entry in google when searching.
- (5) The Subcommittee Commission I.1 of Division I has increasingly been requested to collaborate stringently in decision taking processes of the Interdivisional Committee on Terminology, Nomenclature and Symbols regarding IUPAC adopted terminology, nomenclature and symbols. Also the work of the Subcommittee has been said to be insufficiently reactive to demands for modifications of the Green Book, mainly from other bodies within IUPAC. In the present, project related working principle of IUPAC bodies, it is difficult to reply to these requests. This issue is evoked further below in the specific chapter referring to activities of the Subcommittee.

IV. Project details and publications

After the 95th Bureau Meeting held in Coimbra last year, the following 4 projects were approved and funded.

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 physicochemical 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.

Other current projects are:

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.

Projects that have been concluded since the last report are

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 is up to be published by the Royal Society of Chemistry in 2015.

V. Activities of Commission I.1

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 4th printing, one part of the task group will meet in July 2015, and the Commission will gather at the General Assembly in Busan to finish the preparation of the text to be sent to the publisher for the 4th printing..

The Green Book is being translated into several languages. The Japanese and French translation of the 3rd edition have been published recently. There is a Spanish translation of the 2nd edition. A Turkish and Portuguese translation are in preparation. The Italian translation is finished, but a suitable publishing company has not yet been identified.

The abridged version of the Green Book is technically finished. The missing piece of work is related to the lay out. The print-ready manuscript is expected to be sent to the publisher in 2015.

In addition to its core activity, the Subcommittee has been continuously more requested to collaborate stringently in decision taking processes of the Interdivisional Committee on Terminology, Nomenclature and Symbols regarding IUPAC adopted terminology, nomenclature and symbols, as these are potentially used by economic and political authorities worldwide. Fact is that this Subcommittee has tacitly stopped to meet in its full composition after the General Assembly in Brisbane, in 2001. Meetings have been crucial for the progress of the Subcommittee's work in the past and the lack of meetings is hampering the progress of the work. Unlike the preparation of a specific Recommendation, or Technical Report, the contents of the Green Book involve many facets of physical chemistry. Despite this fact, demands for modifications have continuously been incorporated, i.e. during the several printings of the 3rd edition. However, not all demands can be treated without throughout discussion among Subcommittee members and exchange with groups of experts. For this purpose, regular meetings seem to be essential. In the present, project related working principle of IUPAC bodies, there is hardly space for such meetings. If more reactivity or additional tasks are expected from this Subcommittee, it should receive in some way recurrent financial means for meetings. A very similar conclusion has to be drawn regarding the publication of the Gold Book (see above).