



## **DIVISION OF PHYSICAL AND BIOPHYSICAL CHEMISTRY**

**Progress Report for the IUPAC 104<sup>th</sup> Bureau Meeting 25<sup>th</sup> April 2020**

**Timothy J. Wallington, President**

**10<sup>th</sup> April 2020**

This report contains a summary of the aims, activities and priorities of Division I since the last report to the IUPAC Bureau in April 2019. The report follows the format set out by the IUPAC Secretary-General.

### **I. EXECUTIVE SUMMARY**

Significant progress has been made over the past 2 years in bringing projects under Division I up to date. Seven projects were brought to a successful conclusion over the past year and there are no concerns for the ongoing projects. Division I was well represented at the GA in Paris in July 2019 with 13 representatives and engaged in lively intra- and inter-division discussions as documented in the minutes uploaded to the IUPAC website, <https://iupac.org/wp-content/uploads/2019/12/Division-I-Minutes-2019.pdf>. At the GA, Division I expressed its support for cooperation between IUPAC and OPCW. Such increased cooperation is likely to provide strong impetus for countries to remain with IUPAC and for some countries to rejoin IUPAC. To continue communication and collaboration, Division I held GoToMeeting online conferences in November 2019 and January 2020 and plans further GoToMeeting conferences throughout 2020.

### **II. PLANS AND PRIORITIES**

An essential tool used by IUPAC to promote the common language in science and engineering is via the IUPAC Colour Books. These provide the world's authoritative resource for chemical nomenclature, terminology, and symbols. Terminology definitions published by IUPAC are drafted by international committees of experts in the appropriate chemistry sub-disciplines, and ratified by IUPAC's Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS).

Division I and Commission I.1 have completed the 5<sup>th</sup> edition of the Green Book which is in the hands of reviewers *viz.* *Quantities, Units and Symbols in Physical Chemistry 5<sup>th</sup> ed.* This book

provides a compilation of widely used terms and symbols from many sources together with brief definitions.

Division I shares work on the project to update and digitize the Gold Book (2008) on Chemical Terminology. This is the IUPAC Compendium of Chemical Terminology and is the definitive guide to chemical terminology. Cooperation in the initial stages is by CPCDS, Division V, and Division I. As work moves to the next stage in the next biennium, all IUPAC Divisions and ICTNS will be involved.

### **III. Overall Report of Division I and Commission I.1 activities during 2019-20.**

#### **Division I Aims**

The objectives of the Physical and Biophysical Chemistry Division have not changed since the last report. They are listed on the Division's webpage: <https://iupac.org/who-we-are/divisions/>.

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.

#### **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 physico-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 (2020-2021)**

**Officers:** **President** –Tim Wallington;  
**Vice President** – Pierangelo Metrangolo  
**Secretary** - Attila G. Császár;  
**Past President** – Ron Weir

**Titular Members (6):** Jeremy Frey, Frances Separovic, Zhigang Shuai, Hiroko Tokoro, Ilya Voets, and Angela Wilson.

**Associate Members (6):** Joaquim Faria, Vessala Tsakova, Modou Fall, Seung-Joon Jeon, Theo Kurten, and Luis Montero.

**National Representatives (6):** Ilya Vorotyntsev, Gordana Ciric-Marjanovic, Lynda Ngozi-Olehi, Renata Orikanova, Majdi Hochlaf, and Mohamed Deyab.

**Commission I.1,** whose focus is on Physicochemical Symbols, Terminology, and Units and is responsible for the contents of the Green Book: Chair: J. G. Frey (UK), TMs: Romeu Rocha-Filho (Brazil), Yutaka Koroda (Japan), A. James McQuillan (New Zealand), and NRs: A. A. Milchev (Bulgaria), F. Pavese (Italy), M. Quack (Switzerland) and Ex Officio: Ron Weir.

The Division is supported by an Advisory Subcommittee made up of about 10 scientists renewed in 2019. Its role is to advise on project proposals. It is composed of former Division members and scientists outside IUPAC.

The Rules of Operation for Division I were prepared and they were approved by the IUPAC Executive Committee at the GA (Paris) in July 2019. These rules serve as the working document for the biennium 2020-21 and beyond.

## **DIVISION I/COMMISSION I.1 PROJECTS**

A significant part of the activities is devoted to the identification of and support for projects.

### **Ongoing projects listed in the February 29<sup>th</sup>, 2020 Financial Report are:**

**2007-032-1-100** Marquardt: *Green Book (Abridged version)*

**2011-037-2-100** Bazyleva: *Recommended reference materials for phase equilibrium studies*

**2012-044-1-100** Metrangolo: *Basic terminology of crystal engineering*

**2014-010-1-100** Froba: *Recommendation for the definition, preferred symbols for all transport properties*

**2014-021-1-100** Stohner: *Green Book revision Edition 5*

**2014-028-2-100** Turányi: *Chemical kinetics gas-phase elementary reaction at high temperatures*

**2015-002-2-100** Karger: *Diffusion in non-porous solids*

**2016-031-2-100** McDowell: *Notation and conventions in molecular spectroscopy: Vibrational spectroscopy*

**2017-016-3-100** Wilthan: *ThermoML-2017 Revision of an XML based IUPAC standard for thermodynamic property data*

**2017-021-2-100** Iotti: *Chemical and biochemical thermodynamics reunification*

**2017-024-1-100** Wallington: *Evaluated kinetic data for atmospheric chemistry*

**2019-001-2-100** Frey: *Preparation of the 5th edition of the IUPAC green book*

**2019-013-1-100** Bazyleva: *Good reporting practice for thermophysical and thermochemical property measurements*

**2019-025-1-100** Sander: *Henry's law constants*

**Division I projects completed over the past year are:**

**2006-050-3-100** McQuillan: *Wet surface vibrational spectroscopy experiments*

**2010-048-3-100** Cooke: *Common values of nuclear electric quadrupole coupling terms for appropriate nuclei in functionalized hydrocarbons*

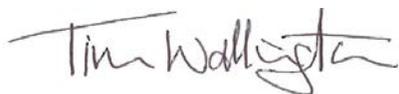
**2012-051-1-100** Fernandez: *International standard for viscosity at temperatures up to 473 K and pressures below 200 MPa*

**2015-038-1-100** Wallington: *Evaluated Kinetic Data for Atmospheric Chemistry*

2016-038-1-100 Rocha: *Quantities, Units and Symbols in Physical Chemistry - Portuguese translation of IUPAC Green Book*

**2018-023-1-FSC** Metrangelo: *14th International Symposium on Macrocyclic and Supramolecular Chemistry (ISMCS2019), Lecce, Italy 2-6 June 2019.*

**2018-005-2-020** Tarasova & Reedijk: *International Year of the Periodic Table of Chemical Elements (IYPT) in 2019: planning, coordination and implementation*



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