



INTERNATIONAL UNION OF  
PURE AND APPLIED CHEMISTRY

## PHYSICAL AND BIOPHYSICAL CHEMISTRY DIVISION

**Progress Report for the IUPAC 105<sup>th</sup> Bureau Meeting August 2021**

**Timothy J. Wallington, President**

**15<sup>th</sup> July 2021**

This report contains a summary of the aims, activities and priorities of Division I since the last report to the IUPAC Bureau in April 2020. The report follows the format set out by the IUPAC Secretary-General.

### **I. EXECUTIVE SUMMARY**

Progress over the past year has been slowed significantly by the pandemic and restrictions in travel. Nevertheless, all projects under Division I have been brought up to date over the past two years. Three projects were brought to a successful conclusion over the past year and there are no significant concerns for the ongoing projects. One new project (2021-006-2-100) has been started in the past year and Division I is contributing to a new project (2021-009-2-500) led by Division V. Elections for officers, TMs, AMs, and NRs for the 2022-2023 biennium were organized and held. Division I held GoToMeeting online meetings in December 2020 and March 2021 and plans a further GoToMeeting call in November 2021.

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

An essential tool used by IUPAC to promote the common language in science and engineering is via the IUPAC Color Books (<https://iupac.org/what-we-do/books/color-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).

Commission I.1 is in the final stages of completing the abridged and the 4th edition of *Quantities, Units and Symbols in Physical Chemistry* (a.k.a. the Green Book). The 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 2020-21.**

#### **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-Cabrera.

**National Representatives (6):** Ilya Vorotyntsev, Gordana Ciric-Marjanovic, Lynda Ngozi-Olehi, Renáta Oriňáková, 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. Its officers are as follows: Chair, J. McQuillan (New Zealand); Secretary, Roberto Maquardt (France); Titular Members, Y. Kuroda (Japan), R. Weir (Canada); Associate Members, S. Chalk (U.S.), G. Deng (China); National Representatives: J. Kaiser (UK), M. Quack (Switzerland); Ex Officio, T. Wallington.

### **Membership (2022-2023)**

**Officers:** **President** – Pierangelo Metrangolo  
**Vice President** – Frances Separovic  
**Secretary** – Attila G. Császár  
**Past President** – Tim Wallington

**Titular Members (6):** Modou Fall, Joaquim Faria, Zhigang Shuai, Ilja Karina Voets, Angela Wilson, and Malgorzata Witko.

**Associate Members (6):** Kwok Feng, Terry Frankcombe, Luis Montero-Cabrera, Igor Schapiro, Hiroko Tokoro, and Vessela Tsakova

**National Representatives (6):** Jeremy Frey, Theo Kurten, Lynda Ngozi-Olehi, Renáta Oriňáková, Vudhichai Parasuk, and Miroslav Štěpánek.

The Division is supported by an Advisory Subcommittee made up of about 10 scientists. 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 May 31<sup>st</sup>, 2021 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*

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

**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*

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

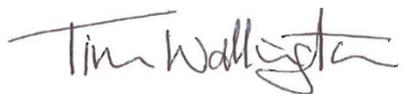
**2021-006-2-100** Resnati: *Categorizing interactions involving Group 11 elements*

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

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

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

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



Timothy J. Wallington, President

Attila G. Császár, Secretary