

DIVISION OF PHYSICAL AND BIOPHYSICAL CHEMISTRY

Minutes of the Division Committee Meeting

**Portinari Room, World Trade Center (WTC), Forum M Level
Sao Paulo, Brazil**

9:00 a.m., July 8, 2017

9:00 a.m., July 9, 2017

Participants:

Angela Wilson (AW, Division I President (DIP), from the US)
Roberto Marquardt (RM, Division I Past-President (DIPP) from France)
Ron Weir (RW, elected TM)
Joaquim de Faria (JF, AM from Portugal)
Pierangelo Metrangolo (PM, TM from Italy)
Ilya Vorotyntsev (IV, Young Observer from Russia)
Modou Fall (MF, NR from Senegal)
Attila G. Császár (AC, TM from Hungary)
Jürgen Stohner (JS, Chair of Commission I.1, Switzerland)
Stuart Chalk (invited guest)
Timothy Wallington (TW, TM from the US)
Jeremy Frey (JF, elected member of Commission I.1)
Frances Separovic (FS, elected TM, joins the Committee for the afternoon of July 8)
Christopher Brett (CB, member of the Bureau, the Executive Office and Chair of Evaluation Committee, joins the meeting in the second day)

Excused: Kristin Bartin (Division Vice-President, Belgium)
Assaf Friedler (Division Secretary, Israel)
Frank van Veggel (TM, Canada)

1. Welcome, introductions, apologies for absences (AW)

AW did not receive a response from Yun Hin Taufiq-Yap and Bert Weckhuysen (BW). Frank van Veggel stepped down as a TM, he announced his absence and is excused. Kristin Bartik and Assaf Friedler accepted to serve in important functions as Vice-Rectors of their universities. They therefore had to present their demission from their current functions as Vice-President and Secretary of the Division, respectively. They announced their absence at the meeting and were excused. AC accepted to write the present minutes.

2. Visit of Secretary General, Richard Hartshorn (9-10 a.m.)

Richard Hartshorn (RH) explains the extended role and the responsibilities of IUPAC in the near future. Summarizes the celebrations connected to the first 100 years of IUPAC (2018). Listens to explanations given by the DIP as to the matter mentioned under item 1. RH reiterates the continuous help from the Secretariat to overcome the difficult situation that the Division has been facing during the last year. He was also sensible to the non-activity of

members and representatives, and said that lack of responsiveness could be sanctioned by the Secretariat.

3. Approval of agenda (AW)

The following item was added to the agenda, suggested by RW: Reunification of chemical and biochemical thermodynamics groups now existing within different divisions.

Decision: The modified agenda was approved unanimously.

4. Recall and approve minutes of the Off-year Division Meeting held in East Lansing, Michigan from August 8-9, 2015 (AW)

PM: Green Chemistry committee must be added to the minutes.

AW: members of different subcommittees must be added to the minutes.

Decision: Approved with the two amendments unanimously.

5. Division I updates – TM/leadership changes (AW)

As reported under item 1, Kristin Bartik and Assaf Friedler will not serve Div. I in the next biennium.

Ron Weir, who led ICTNS for eight years and who stops this activity at the end of 2017, accepted to serve as the next DIP. RW has a long experience with IUPAC, in particular he chaired Division in the biennium 2004/2005.

Tim Wallington agreed to serve as DIVP for the next biennium.

Attila Császár agreed to serve as DIS for the next biennium.

As DIPP, RM would normally have finished his activities within the Division; however, being eligible, he continues to serve Division I as TM in the next biennium.

6. Election results (RM)

RM: under normal circumstances DIPP is the Chair of the Nominating Committee which selects candidates out of the several nominations received from the National Adhering Organisations (NAO); as mentioned under item 5, in order to secure continuity, RM agreed to stay as TM of the Division; Jim McQuillan (JM) accepted to chair the Nominating Committee in his place.

The final nominating committee: Jim McQuillan (chair), Kristin Bartik, Roberto Marquardt, and Romeu Rocha (Brazil). Zhigang (China) was asked to leave as he was himself candidate. RM calls the attention to a new and odd problem: current TM are newly put to be (re)elected; however, what happens to current members if they are not elected?

There have been 10 nominations as TM. The committee made the four groups: experimental spectroscopy and kinetics, material sciences, theoretical and bio- physical chemistry, electrochemistry and thermochemistry. These were on the ballot, on which it was mentioned that two officers step down and continuity is of high priority.

Outcome of ballot: AC, BW, TW, PM, and RM confirmed as TM. Newly elected members: Hiroko Tokoro, JF, FS, and RW.

Vote on further Div. I members for next biennium:

AM

- 6 Associate members are allowed for the next biennium

- 3 remaining members: Vladislav Tomisic, Croatia; Michal Korenko, Slovakia; Theo Christian Kurten, Finland
- The Nominating Committee proposed: Modou Fall (Senegal), Luis-Alberto Cabrera (Cuba), Zhigang Shuai (China)
- Important information: Supa Hannongbua's name was not on the ballot, though she submitted a candidature to Lynn Soby, but there was a miscommunication. DIP will contact the Secretary about this issue
- Decision: all Committee members support the selection of the three AMs

NR

- 3 will stay (Leticia Gonzalez (Austria), Seung-Joon Jeon (Korea), Chia-Chun Jay (Taiwan), no vote is needed
- 7 suggestions from JM: Joaquim de Faria (Portugal, spectroscopy and photochemistry), Keith Gordon (NZ, spectroscopy), Gamini Rajapakse (Sri Lanka, materials, electrochemistry), Vessela Tsakova (Bulgaria, electrochemistry), Ioanna Zoi (Greece, quantum mechanics of biomolecules), Malgorzata Witko (Poland, quantum chemistry), Ilya Vorotyntsiyev (Russian Federation, analytical chemistry)

A discussion followed about the participation of members at divisional activities.

Decision: to review the position of TM, who never showed up at Div. I events.

7. **Reunification of chemical and biochemical thermodynamics groups now existing within different divisions (RW)**

Decision: Following a discussion led by RW all agreed that this is an important issue and the discussion should continue once old related documents (to be sent around by RW and RM) and discussions are revisited.

Decision: All agreed that we do need to bring IUBNB and IUPAC together. Persons suggested to be contacted: Gerry Moss and Bob Goldberg.

8. **A brief overview of division work, aims, and objectives (AW)**

RW: processes have changed about the election rules. RM: suggests to help IUPAC to make the election process better the next time around.

RM: separate regular (administrative and practical) work from scientific work of Div. I.

MF: French is the official language in Senegal, Ministry of Education in Senegal seeks IUPAC approval of French textbooks written in French by local authors. AW and RM: this is outside of the responsibility of IUPAC divisions. Decision: All agree that no action should be taken.

RM: the official language of IUPAC is English; he mentions the translation of the Green Book into French and Portuguese, the latter is up to be published, and points out that these books were not reviewed by ICTNS, hence they are not official IUPAC recommendations; however, as their production benefited from the direct supervision of Commission I.1, their visibility as IUPAC related documents in the corresponding language specific regions of the world will probably be very high.

JS: Div. I should put a contact person on the IUPAC website for Task Group projects.

RM: should go back to the monitoring system which existed before the last biennium; reinvestigate how the committee works; initiates regular phone meetings about committee

activities (e.g., once a quarter); RW: this could be done through IUPAC Secretariat. AW: will put together a draft about roles of committee members, based on an earlier document of JM. Decision: continue discussion the next day based on a preliminary draft.

AW: suggests a phone meeting in October 2017. Decision: supported unanimously.

AW: in 2020 organize, before Pacifichem (Honolulu), an off-year meeting (around 15 December 2020).

The 2019 meeting will be in Paris.

A longer discussion about the role of ICTNS in relation to documents (e.g., IUPAC-approved books). Following a discussion led by RM and JS all agreed to the following: a very clear timeline must be set; reconsider the role of ICTNS; publishers must be aware of IUPAC policy about providing IUPAC approval on book projects; it is hard to find scientific reviewers, a book chapter needs on average a month to be reviewed; all divisions must see the documents so that they can express their opinion (this is a lengthy process); division presidents should see the contract with the publisher before agreeing to support a project; the role of the divisions and of ICTNS as reviewers must be part of the book contract; ICTNS must receive approval of division decisions prior to its handling of books and documents; the reviewing process and regular IUPAC processes should be disentangled; contracts should be the same for all divisions; royalty distribution should be made clear and transparent. AW: part of the money should go back to the Division backing the document (notes good related ACS practice).

9. Discussion of Committee tasks, responsibilities, web site, project monitoring, etc. (AW/RM)

RM: One Committee person should deal with the website (they use WordPress), used to be done by Frank. Decision: accepted the volunteer help of JF to become web manager in the future. Note added in proofreading: RM takes the responsibility as website manager of the Division, as JF will be busy with Commission I.1 business.

RM and JF: Activities of the Committee should be present on the website. Kristin used to communicate with Lynn about changes but progress has usually been slow. Lynn would like to control strategic decisions about the website, which is supported.

RM: color books are still not visible properly on the official IUPAC website.

AW: Div. I needs a project manager, perhaps Tim can be asked to do this. RM: very reasonable that the DIVP takes this duty. Decision: include this task in the Operating Procedures.

AW: need people assigned to different committees. The present list is as follows: ICTNS: Roberto, Ron; Inorganic: Materials: Angela used to do this, Joaquim goes on Monday; CPCDS: RW; CCE: Modou Fall will take over.

AW: would be nice to have an internal, password protected website for the Division to put documents on for the future.

JF: volunteers to set up an internal website where internal documents could be stored (these could be accessed from Minutes)

10. Visit from the chair and secretary of the Committee on Chemistry Education (CCE)

Jan Apotheker is the current secretary of CCE, while Mustafa Sozbilir is current chair. Jan Apotheker and Mustafa Sozbilir address the Committee Meeting, noting that they are going

around in divisions to see if there are new cooperation possibilities. CCE is willing to support joint projects on chemical education (have several joint projects with Div. II).

Mustafa Sozbilir advertises the Flying Chemistry Educators (FCE) program, going to underdeveloped countries (teacher education, research education, local organizer has to support partially the mission), last one organized in the Pacific Islands, involving workshops and training activities. RW: need education articles about the Mole project; is there a role for CCE in this? Mustafa Sozbilir: Marcy Towns was brought to Mole project. RM suggests to write articles in individual countries about the project (including translation of recommendations).

RM: one possible Div. I project is on the use of absorption intensities, this is related to education. Mustafa Sozbilir: send a note to Suzanne Boniface, currently secretary of CCE, as some CCE members may be interested.

Jan Apotheker takes the opportunity to promote the 2023 GA event in NL.

11. Revisit the list of the Div. I Advisory Board (AW)

Decision: The Committee agrees to the following: terms should be implemented; the Advisory Board (DIAB) has an important role with respect to projects coming in; the present size of the DIAB is too large; the DIAB could advise on future activities of Div. I; the activities of the DIAB should be reviewed for every biennium.

Decision: The following persons should be approached by the DIP to form the new DIAB: Christopher Brett, Robin Harris, Michael Frenkel, Henrik Kjaergaard, Katharina Kohse-Hoeninghaus, Ruth Lynden-Bell, Jürgen Troe, Sally Price, Gerry Moss, Supa Hannongbua, Kalina Hristova, Bonnie Wallace, and Lucie Carpenter.

12. Student cartoon competition and going forward (RM)

RM: The action was very disappointing despite thorough preparation. No entries were received.

Decision: All agree that this competition should be continued. Help from CCE should be sought. RM volunteers to discuss setting up a subcommittee between Div. I and CCE.

IV offers to send a document to all Committee members about a good practice in Russia.

13. Semantic units for digital applications (Stuart Chalk, University of North Florida, USA; <https://units.unf.edu>)

The detailed presentation was followed by a discussion. The Committee discussed the advantages and the dangers if units and symbols are computerized and not dealt with by humans. The discussion extended to the implication of this action in IUPAC projects involving xml versions of the color books, and the Gold Book in particular. The committee is very interested in pursuing the connection with Dr. Chalk and to continue to be informed about the progresses made in his project.

14. Future Div. I activities (AW)

AW: separate the discussion of activities from that of future projects.

Possible future activities: IUPAC symposium at a PacifiChem meeting and a video competition.

JS brings up the question of wrong past recommendations. Suggests to scan old recommendations for inconsistencies or errors to avoid the problems in the future. Div. I should be looking for outdated recommendations, as well.

AW and RM: Franco Pavese could be one possible project leader.

Decision: JS is asked to approach Franco Pavese.

PM would like to receive support from Div. I to endorse a conference he's organizing in Lecce on Supramolecular Chemistry (an emerging field).

RM: Div. I could sponsor a poster prize (300 USD).

AW: which meeting and why support a particular conference.

Decision: no support is offered.

PM: IUPAC could perhaps approach Cambridge Database (and perhaps other vendors) to set data standards.

JS: IUCr is well linked with IUPAC.

AW: linking to other professional societies?

JF: interesting project would be the link between biological systems overlapping with physico-chemical ones.

15. New project proposals (AW)

RM: a project about spectroscopic line intensities. RM cannot lead the project, Joaquim said he could do that.

PM: big data project.

AW: one of top ten topics for NSF (terms "data science" and "data discovery" is used instead of "big data"). We are often not sure how to use data.

RM: in chemistry we often have "not constant" data, which gets improved over time (put on cloud).

JF: CODATA is an interunion force, CODATA is taking the lead. What exactly can Div. I do about data?

RM: truthfulness, respecting standards, units, format, good practice.

JF: IUPAC could suggest projects to CODATA, which is a good vehicle to such projects.

Chris Brett may have a project for the Division about electrochemistry (corrosion chemists and corrosion engineers should share a common language).

Chris Brett: there will be a green chemistry project asking for support from different divisions.

TW: going to propose a new project (up to 19000 USD)

RM: Commission I.1 is another standard project of Div. I which receives support of 10000 USD per biennium.

Second day of the meeting (July 9)

Participants:

Angela Wilson (AW)

Joaquim de Faria (JF)

Pierangelo Metrangolo (PM)

Attila G. Császár (AC)

Roberto Marquardt (RM)

Supa Hannungboa (SH, NR)

Chris Brett joins the meeting after the first break

Zhigang Shuai joins the meeting after the first break

Mary Garson joins briefly the Committee meeting and talks about IUPAC100 (2019)

16. Project reports (AW)

2006-050-3-100 (Surface Vibrational Spectroscopy Experiments) – Jim McQuillan

there is still money left on the account (about 3200 USD)

justification of continued work: Jim gave solid arguments to continue the project; he is not sure whether the remaining money will be used

Decision: grant him permission to continue and to report, until next the off-year meeting, whether and how the money will be used.

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

not much work left

will be finished by end of August 2017

120 pages document is basically ready

most of the work was done by Jürgen

Decision: grant no-cost extension until the next off year-meeting

2007-055-2-100 (Ultrafast Intense Laser Chemistry) – Kaoru Yamanouchi

Kaoru has a rough draft, but no real document

AW has not seen any documents

Decision: no-cost extension granted and request to send a draft by the next off-year meeting

2010-009-1-100 (Physisorption of Gases, with special reference to the evaluation of surface area and pore size distribution) – Matthias Thommes

This project was successfully completed in 2015 (see minutes of the Busan meeting 2015, already uploaded on the web). The remaining funds of USD 1572 return to central.

Decision: recall 2015 decision and send remaining funds of USD 1572 to central.

2010-048-3-100 (Common Values of Nuclear Electric Quadrupole Coupling Terms of Appropriate Nuclei in Functionalized Hydrocarbons) – Stephen Cooke

AW: should be terminated, one-person project instead of collaboration, no response.

Joaquim Faria: Criteria for authorizing the continuation of a project should be reviewed and tightened.

Decision: the project is **terminated and non-used funds of 1000 USD will be returned to central.**

2011-037-2-100 (Recommended Reference Materials for Phase Equilibrium Studies) – Ala Bazyleva (Robert Chirico)

This project was terminated at the 2016 off-year meeting.

Decision: recall 2016 decision and send remaining funds of USD 11 000 to central.

2012-044-1-100 (Basic Terminology of Crystal Engineering) – Pierangelo Metrangolo

PM: Started March 2013, budget increased by ICSU, selected 22-30 terms, now list of 22 plus additional 8, more than 50 people were interviewed, these 30 terms are essential; 9 terms are completed (2 pages, plus history, normal use, etc.), take inactive people out if they do not answer, 6 people in the Core Group. The aim of the project was to provide clarity for technical definitions in the form of an IUPAC recommendation.

RM: Could some of the terms be reduced? Budget-wise it's ok.

Decision: The project will be continued.

2012-051-1-100 (International standard for viscosity at temperatures up to 473 K and pressures below 200 MPa) – Josefa Fernandez Perez

This project has also started by Tony Goodwin.

AW: will contact TG lead

Decision: The project may continue, given the special circumstances, but a clear report is needed before the next off-year meeting.

2013-003-3-100 (Experimental Thermodynamics Volume IX: B, Non-Equilibrium Thermodynamics and Applications) - William Wakeham

This book project was successfully completed in 2016. The remaining unused funds of USD 4 700 will return to central.

Decision: successful completion, AW writes to secretariat and returns remaining funds.

2013-048-1-100 (A Critical Review of the Proposed Definitions of Fundamental Chemical Quantities and their Impact on Chemical Communities) – Jürgen Stohner

RM: Jürgen will report today about the progress on the joint meeting with Divs II, V, CCE, ICTNS (see item 19 below). This project was a complete success. It is a highlight project of the Division in the past two years.

Decision: This project is considered complete.

2014-010-1-100 (Recommendation for the Definition, Preferred Symbol for All Transport Properties) – R. Banish

No response has been received from the TG Chair, another email was sent out. No money has been spent on this project so far.

AW: TG Chair promised a report but it was not delivered after the East Lansing meeting. See also Busan note.

RM: Angela should ask him whether we should close this project.

Decision: give 4 weeks, the grant is frozen for the moment, we'll discuss at the next meeting.

2014-021-1-100 (Green Book revision) – Jürgen Stohner

RM: gives a brief account about the progress on project, Jeremy accepted to lead this project, Jeremy will lead the new project, Commission I.1 should have some reserved money, at the moment no money is needed but Angela asks Roberto to commission the money, the future DIP (Ron Weir) should remember this.

AW: Div. I continues to fund the work of Commission I.1.

Decision: A further discussion of this project will be given at the next off-year meeting; remaining funds can be used.

2014-028-2-100 (Chemical Kinetics of Gas-phase Elementary Reactions at High Temperature) – Tamas Turanyi

AW: gives a summary.

RM: check for overlap (constructive is good) with Tim Wallington as he also works on kinetic data.

AC: explains the DOI associated with the representation of data in individual papers.

Decision: the project can go on, a comparison between this project and project 2015-038-1-100 should be made and discussed by the Committee latest at the next off-year meeting.

2015-002-2-100 (Diffusion in Nonporous Solids) – Rustem Valiullin

AW: one publication in Sci. Rep., 3 common names from TG membership and authorship of this research paper.

AW: include the notes as an appendix to the Minutes for all TGs.

RM: remind the TG leader that the Division expects a recommendation or a technical report as a result of the TG work.

Decision: the project can continue, AW reminds the TG lead that a technical report or a recommendation are expected outcomes from the project.

2015-038-1-100 (Evaluated Kinetic Data for Atmospheric Chemistry) – Tim Wallington

This project has made good progress. Details are in the project report file.

AW: IUPAC should manage websites containing the data.

RM: IUPAC had problems with websites, should be overviewed by Division I, Committee keeps access to the database created.

Decision: the project can continue, a comparison between this project and project 2014-028-2-100 should be made and discussed by the Committee latest at the next off-year meeting.

2016-031-2-100 (Notations and Conventions in Molecular Spectroscopy: Rotation-Vibration Spectroscopy) – Robin McDowell

Division I sponsors alone the project with 250 USD.

RM: This project is an important continuation and consolidation of two former IUPAC recommendations on high resolution spectroscopy.

Decision: The project can go on.

2016-038-1-100 (Quantities, Units, and Symbols in Physical Chemistry - Portuguese Translation of IUPAC's Green Book – Romeo Rocha-Filho

Joaquim Faria: Portuguese translation of Green Book experiences a problem, the index costs more (translation of index costs more).

RM: doing layout and cover page, original plan was to present it at the meeting, but due to technical difficulties with the indexing of terms and symbols, its submission had to be delayed. Funds will be used to pay a company which provided professional technical support in hosting and managing the LaTeX files needed for the compilation. The TG will keep control of all files produced. An xml version of the book is planned, which is of interest to Commission I.1 for its own xml related work on the original version of the GB.

Decision: This project can continue, the so far allocated money can be used, but no further financial support will be given by Division I.

2016-001-2-300 (Categorizing Chalcogen, Pnictogen, and Tetrel Bonds, and Other Interactions Involving Groups 14-16 Elements) - Giuseppe Resnati

Div. I committed 4000 USD, but Division III is the leading division; no project report was delivered.

PM: also co-leader but has no updates at this moment.

AW: Angela will send out an e-mail and request a report for the next meeting.

Decision: the project can continue.

17. Budget

AW: summarizes the budget items for 2016/17. Remaining balance is almost 32000 USD.

RM: recalls JF and JS to submit a request to commit money for the next biennium for Commission I.1.

RM: Ron is reminded of the Commission I.1 project.

RM+Joaquim: project on line intensities, recommendation on “line strength”, “absorption cross section”, “epsilon”. Some colleagues from CCE should be involved (Edit Mátyus could be involved).

Laura McDowell (PP of Div VI): Workshop in December 2017 about water management.

RM: asks Supa and Zhigang (elected AM member of Div. I) to submit a proposal.

At this point the Committee interrupts its meeting and joins the cross-divisional meeting on the “mole”-project, which will be in room Monet, starting at 11:30.

18. Next off-year meeting

AW: preferably it should be in the EU to reduce cost. PM offers to have it in Milan. Planned date of the 2.5 day meeting, with small conference: summer (June-August 2018).

Decision: AW should set up a doodle poll about the best weeks.

19. Cross division session on the mole (11:30-12:15, Sunday, July 9 in Monet room)

All Committee members participated. JS gave a detailed presentation of the project, its results and the forthcoming actions with IUPAC involvement in the new SI definitions.

20. Other

A draft of "Operating Procedures" was presented by AW and discussed. Its approved structure is as follows:

- I. Mission, objectives, and aims
- II. Management
- III. Composition
- IV. Membership and appointments
- V. Nominations
- VI. Elections
- VII. Officers
- VIII. Executive and term of office
- IX. Subsidiary bodies

All agreed that once the document is finalized it should be put on the Div. I website.

All agreed that DIP should approach the Secretariat about lack of instructions regarding quorum and proxy in the 2016 Bylaws.

RM suggests to prepare a special event for the World Congress in Paris, honoring Jean Perrin. Decision: RM organizes this mini-symposium, Div. I should set money aside for this.

JF: Palais de la découverte could be the place to organize the mini-symposium.

FS: only living female chemistry Nobel Laureate (special issue in PAC) should also be celebrated.

RM: who'll organize the PChem meeting in Paris? Will ask Jean-Pierre Vairon.