

Division I - Off year meeting, August 26-27, 2016, East Lansing MI, USA

Participants:

Angela Wilson

Assaf Friedler

Kristin Bartik

Jurgen Stohner

Frank Van Veggel

Pierangelo Metrangolo

Roberto Marquardt

Tim Wallington

Attila Csaszar

Luis Montero Cabrera

Excused:

Taufiq Yap Yun Hin

Bert Weckhuysen

1. Welcome and introduction, agenda

The following items were added to the agenda: discussion of website, whether nomenclature should stay in the division aims, the role of young observers, book projects

2. Approval of the Busan Minutes

Corrected minutes approved

3. Cartoon competition: (discussion took place over the two days)

The history of the competition was described. RM suggests that for next year in Brazil the competition could focus on high school students from the greater Sao Paulo area. The best ones will be invited to the IUPAC meeting to participate and get the prize. The idea of a video competition was also raised. The cartoon should be in English.

Decision: RM will run the cartoon competition this year. Two modes are proposed:

1. Worldwide cartoon competition for undergraduate university students. The cartoon will be related to the theme of the IUPAC congress: What biophysical chemistry represents and what is its role for the environment and living bodies.
2. High school students from the Sao Paulo area, where the theme will be chemistry in general.

Proposed Awards: for the worldwide competition an invitation to the congress. We should ask for 3000 USD from the returned money for that.

For the local cartoon – the prize will be an invitation to the congress for the three first winners and a money prize (50, 100, 150\$).

Action: AW will contact the organizers of the IUPAC meeting and will also speak with the editor of JPC to enquire about the possibility of displaying the cartoons in the journal

4. General policy about book projects:

KB reviewed the history of book projects in the division. RM said that a peer review procedure is missing for books. The new contract that IUPAC has established with the publisher was sent to everyone. JS suggests a discussion among all division presidents. RM said that the issue was indeed already discussed in such a forum and the secretary general gave more attention that the royalties issue be solved. The royalties issue is indeed solved but other issues remain open, such as the peer reviewing procedure.

A major issue raised is the time needed for the review. This was not solved yet. JS said that the project proposal should pass between the divisions and ICTNS and only then contracts with publishers should be signed. KB on the other hand believes that the contract should be signed at the beginning. The idea was raised to add in the contract that the publisher must send the chapters for external review and that the reviews should then be sent with the chapters to the Division and ICTNS. If the reviews are not good enough we will remove the IUPAC logo. In any case, the division presidents should view the contracts before they are signed.

AF suggested that we tell Fabienne that while we are happy that the royalties issue was solved, we are still concerned about the review timeline and quality control. We need time for the reviewing and we need to also have the chance to re-review after the corrections are introduced, which should take together up to three months. RM emphasized we should ask for enough time for the reviewing.

To summarize this point, the division committee raises a question about a general IUPAC policy about books. Two issues are remaining to be solved: 1) Quality control and 2) how the money is used since as opposed to standard projects, the money here is not intended to bring a task group together.

Decision: It was decided that division committee I does not approve book projects for the time being and will review book projects only if the two above issues are resolved.

Action item: AW will inform the secretariat that we do not approve book projects now. We might accept them in the future only if the contract will specify that the IUPAC label is provided only if the scientific review is satisfactory according to the division.

5. Skype call with Mark Cesa:

A skype call was conducted with Mark Cesa, in which he updated the division committee about the topics discussed and decisions made in the last bureau meeting. Among the topics raised:

- -international young chemists network would like to join IUPAC. The concept was endorsed.
- -updates about grant proposals to ICSU together with the unions of physics and math
- -a new membership relations committee
- -new interdivisional committee on green chemistry
- -management committee for the IUPAC centenary was established

RM asked if the new definition of the mole was discussed. Answer is no.

FvV asked about conflicts between codes of conduct between IUPAC and the societies.

AW raised the book projects issue. Mark said that other divisions might experience similar problems and agreed that the problem should indeed be sorted out. Mark asked for something written to bring to the EC.

AW raised the world congress and lack of involvement of DCs in it. Mark asked for specific examples. He said that the IUPAC policy is not to be involved in organizing apart from advising. AW suggested that each DC should be given the opportunity to organize one symposium.

6. Updates on projects:

The division committee decided to continue using the new project reporting form initiated this year and have a regular due date for reports (July 15 is suggested). The Division has also agreed to go to once-per-year due dates project submission and the IUPAC management will be consulted to see whether and how this is possible.

The updated information about the projects, based on the reports of the task group leaders, was presented by AF:

2006-050-3-100 – McQuillan

Manuscript expected by the end of the year. The project is progressing, though slow. They do plan to finish the project.

Decision: Grant a no-cost extension until July 2017, and discuss again in Brazil.

The project still has ~\$3K remaining. AW will write to the task group leader, asking that if the funding is not intended to be used, we would like to pull it back into IUPAC.

2007-032-1-100 – Marquardt

Green Book – Abridged version.

RM reported on the project. The content of Green Book is there. Only Roberto and Jurgen are working on it. Not expected in 2016 but they hope to have it done for 2017.

Decision: Grant a no-cost extension until July 2017, and discuss again in Brazil.

2007-055-2-100 – Yamanouchi

Did not respond to report request. AF will send a reminder and say that we hope that he will finish the project.

Decision: Grant a final no-cost extension until July 2017.

2010-048-3-100 – Cooke

Project is stalled – they are getting personnel to complete the project.

Decision: Grant a final one year no-cost extension

2011-037-2-100 – Chirico

No answer for a couple of years in a row.

Decision: terminate project - \$11,000 left should be returned to the central budget.

2012-044-1-100 – Metroangelo

PM reported on the progress of the project. The task group received also ICSU funding. They created a list of 30 terms essential to crystal engineering and are now working on the definitions. They will meet in Milan around April 2017 to present the

results to a panel of experts. This is a joint project with IUCR and it will be presented to IUCR in a special symposium on crystal engineering at the IUCR meeting in 2017.

Decision: a no-cost extension until end of 2017 was granted.

2012-051-1-100 – Fernandez Perez

This is the project that Tony Goodwin was leading before his untimely death, and was taken over by one of the task group members. The project is making good progress.

Decision: a no-cost extension until end of 2017 was granted.

2013-003-3-100 – Wakeham

Project is now completed. The remaining funds will return to IUPAC.

2013-035-1-100 – Wallington

Project is completed.

2015-038-1-100 – Wallington

TW reported on the project, which is making good progress. A compendium of kinetic parameters is being worked on.

2013-048-1-100 – Stohner

JS reported on the project. A manuscript has been submitted and they are now waiting for the referees' reports. See details in item 16 below.

A one year no cost extension was granted.

2014-010-1-100 – Banish

The task group leader promised to send a report in a few weeks.

2014-021-1-100 – Stohner

JS reported on the project. Roberto recalled the point already discussed and decided in the last meeting, that Commission 1.1 should have recurring funding for each biennium for the work on the Green Book.

2014-028-2-100 – Turanyi

Good progress is being made

2015-002-2-100 – Valiullin

Making good progress.

2015-002-2-100 – Lechter

Making good progress. Plans to be done by August 2017

The Resnati project **2016-001-2-300**, which we support with 4000\$, should be added to our list.

The issue of deciding about approval of new projects was raised. It was decided that the review process should be managed centrally by Fabienne. Project proposals should be submitted to Fabienne, who sends to DC officers (president, vice-president and secretary). They tell her who the external reviewers should be. Fabienne will then send for external review and when she has received them, send the proposal and the review reports to all the DC members. The DC members will give their opinions about the approval of the project to the secretary and president and the president will take the final decision.

Decision: to have one deadline each year for project submissions and decisions will be made during the off year or annual meeting. The actual deadline should be decided and the idea discussed with Fabienne.

Action: AW will contact Fabienne to outline the procedure and also see if a single deadline per year is possible.

7. Future projects and emerging areas of importance:

AW raised the issue of chemical informatics and databases: How to utilize and manage data and how to deal with heterogeneous data. PM suggested the topic of big data.

TW suggested a theme related to transparency and reproducibility of data.

RM mentioned the six points raised in the 2014 Switzerland off year meeting. The question is how to encourage people to pursue projects.

AW suggested writing on the website which type of projects we are interested in. Someone should be in charge of delivering the content for the website.

RM suggested appointing a liaison to IUPAP

The interdisciplinary nature of chemistry was discussed and the issue of a new DC about chemical biology was raised again. A subcommittee is not the best case since they have no funding (see the materials chemistry subdivision as example). We should be more involved with chemical biology projects that are being funded in other divisions. PM suggests adding to the project form a primary and secondary division.

Action items: Angela will speak with the presidents of other relevant divisions and say we would like to be involved in biophysical projects (including financial support). Express our interests more clearly on our website. KB will ensure that this is done.

JS reminds us that Div1.1 should review each project that is related to terminology

8. Role of IUPAC titular members:

AW reviewed the roles of TMs: evaluating new projects, special roles like the website etc., having a critical view of ongoing projects, think of new projects, Liaisons with other divisions.

Liaisons list:

Roberto – division 2

Pierangelo –division 3

Frank – division 5

Tim –division 6

Assaf – division 7

RM went over the list of division representatives from last time and explained how the system works in this regard.

9. Division 1 – our role as a division

The discussion was about additional activities, in addition to the projects and cartoon competition. It was decided that the division should aim at organizing sessions in the

IUPAC conference and in other conferences that have the IUPAC label. AW will look into how to do it.

10. Advisory board:

The advisory subcommittee should be updated: RM will go over it and send to KB, who will finalize. The terminology will change from "advisory board" to "expert list". Angela will inform the central office.

Several participants said that the advisory board has no function and should be removed completely. This will be discussed in the future

11. Website:

KB rephrased the division aims for the website and the text was approved by the Division.

Suggested changes/updates:

- all meeting minutes and presidents reports should be made available on the website
- The cartoon competition should appear under a different title with a link. The current link is wrong.
- Colour books should have a link directly from the main page – from "what we do" add a link to colour books
- "physical and biophysical chemistry" should be used at all times to refer to our division (the term biophysical is missing in certain links).

Action items:

- -AW will email Fabienne saying that IUPAC should not put information about the division without us looking at it before.
- The new text for the aims will be emailed to Fabienne to be put on the website.
- -AF will send all the old minutes. AW and RM will send the presidents reports.
- -AF will request that they add links to our projects
- -JS will send the correct pdf version of the green book

- Members list will be updated and corrected and sent to everyone

12. Young observers:

RM and TW volunteered to guide the young observers in the next meeting

13. Translation of the green book:

The project of translation of the green book into Portuguese is almost complete. The translation is finished. 3000 Euro are required to pay a company that hosts the site for the book. RM asks that if there is division money left we could use it. The division approves.

Action item: RM will email the central office about it.

14. Elections:

RM explained the election procedure. Discussion was in which fields we need new TMs. Fields that are missing are thermochemistry, electrochemistry. Also need someone from industry.

Office for next biennium:

Angela Wilson – Past President

Kristin Bartik– President

Assaf Friedler– Vice President

Frank Van Veggel – Secretary

15. The mole project:

JS and RM updated about project 2013-048-1-100 ("the mole project"). In the proposed new SI, the kilogram will be redefined in terms of the Planck constant and the mole will be redefined in terms of the Avogadro constant. These redefinitions will have some consequences for measurements in chemistry. The goal of the Mole Project was to compile existing published work related to the definition of the quantity 'amount of substance', its unit the 'mole', and the consequence of these definitions on the unit of the quantity mass, the kilogram. The published work has been reviewed critically with the aim of assembling all possible aspects in order to

enable IUPAC to judge the adequateness of the existing definitions or new proposals. Compilation and critical review relies on the broadest spectrum of interested IUPAC members. A manuscript was submitted as an IUPAC Technical Report to all Divisions and IUPAC National Adhering Organizations. The Task Group managed to come up with a new definition of the mole. This should be prepared as an IUPAC Recommendation to be submitted as soon as possible.

The division approved its support for the new proposed definition and would like IUPAC to propose the new wording to the CCU. JS will write to the bureau asking to approach CCU with this wording.