

**IUPAC Division Committee I**  
**Minutes of the off year meeting 2014**

The 2014 off-year meeting was held at the Kloster-Kappel hotel, Kappel-Am-Albis, Switzerland, on the 31.5 – 1.6. 2014

**Present at all discussions were:**

Roberto Marquardt (President)

Kaoru Yamanouchi (Past president)

Angela Wilson (Vice president)

Assaf Friedler (Secretary)

Kristin Bartik (TM)

Anthony Goodwin (TM)

Jürgen Stohner (TM)

Frank Van Veggel (TM)

Taufiq Yap Yun-Hin (TM)

Attila G. Császár (AM)

Kankan Bhattacharyya (AM)

**1. Welcome and apologies (RM):**

The President welcomed the division committee members and sent the apologies by Andrea Russell for not being able to participate in the meeting. The President sent greetings to the new DC members.

**2. Agenda (RM):**

1. Welcome, apologies for absence (RM)
2. Approval of Agenda (RM)
3. Recall and approval of Minutes of the Division Meeting held at the Harbiye Military Museum in Istanbul, Turkey, from August 9-10, 2013. (AKW/AF/RM)
4. A brief recall to the Divisional work, its aims and objectives (RM)
5. A brief report from the Bureau meeting in Coimbra (RM)
6. Progress Reports on Current Projects (AF)
7. Finances (AF/AKW/RM)
8. Future Strategy and New Project Proposals (RM)

Discussion on the six topics proposed in Istanbul (biophysical, shale gas, light absorption intensity, data standardization, materials, density functional theory) and potential new proposals. Involvement of committee members or other IUPAC fellows.

9. Discussion about IUPAC or Division Activities related to the forthcoming International Year of Light, 2015 ([http://www.eps.org/?page=event\\_iyol](http://www.eps.org/?page=event_iyol)) (RM)

10.. Discussion of sharing of Committee Tasks/Responsibilities (AF/RM/KY): Involvement of NAO; the concept of a “Division liaison”; web responsible; newsletter responsible.

11. Miscellanea

replicate publications in PAC

12. Elections for the next biennium (KY/RM)

13. 48<sup>th</sup> GA (Aug. 6-13) and 45<sup>th</sup> Congress (Aug. 9-14), 2015 Korea (<http://www.iupac2015.org>)

Discussion about BPC symposium and other business.

14. 49<sup>th</sup> GA and 46<sup>th</sup> Congress in Brazil, 2017

Divisional involvement, co-organization of the BPC symposium

- JS suggested adding to point 11 of the Agenda: discussing a suggested change in the IUPAC bylaw about length of membership
- RM suggested two additions:
  - royalties about IUPAC publications should be discussed when discussing ongoing projects
  - possible modifications of the division aims

Modified agenda approved unanimously.

3. **Minutes of the 2013 Istanbul DC meeting (AKW, AF and RM):** It was noted that 2012 should be corrected to 2013 in line 1. Correction was made and the minutes approved.

4. **A brief recall to the Divisional work, its aims and objectives (RM):** The president described the division aims, objectives and work based on the report submitted to the bureau (pages 1-2). The report was emailed to the DC members.

5. **A brief report from the Bureau meeting in Coimbra (RM):** The meeting took place in Coimbra on April 12-14, 2014. A meeting of division presidents took place on the 11.4.2014. A meeting of the IUPAC web vision team also took place. Division 1 was assigned to the membership committee (seeking new NAOs). There are very few members from sub-Saharan Africa and division 1 is in charge of finding new connections in Africa. DC members are asked to try and report about such connections within 3 months. RM will try to make connections with North Africa. Kankan will look at possible ideas being an editor of JPC. Taufiq-Yap mentioned

South East Asia. Roberto answered that other divisions are assigned for SE Asia and the Arab world. DC I is in charge of Africa.

RM reported about several points that were raised in the meetings in Coimbra, and some of them were discussed as detailed below:

- In the meeting of division presidents there was a discussion of interdivisional liaisons (item 10 on the agenda).
- DC 1 will receive new instructions for election timeline
- A new color book integration project was initiated: The idea is to make all the color books e-books using a new content management system. Mark Kinnan is in charge. JS is in charge of it from our division.
- The PAC editor suggested publishing conference special issues in PAC. A discussion was made whether and how this is possible. Committee members are encouraged to send ideas. AC said that the publication process is very difficult. RM said that there were problems while changing publisher but these are solved now. There are problems with the review process.

Report of RM from the bureau meeting:

- Since September 2013 IUPAC has no executive director. There is a search for candidates. IUPAC members should know the reasons for ED changes
- Colin Humphries is the new secretary general
- The current vice-president, Prof. Natalia Tarasova, explained her strategic views of IUPAC's future: What is chemical pollution? What are the needs? What can IUPAC do to meet the needs? Tight up involvement with ICSU (International Council for Sciences).
- The division presidents presented their reports. Division 4 reported an agreement about royalties when a project is published as a book. RM will find out the details for implementing in our DC as well.
- Two new interdivisional committees were established: the gold book committee and wiki-survey.
- Transition of PAC to De Gruyter was discussed. There is a new team that will interfere with De Gruyter, under CPCDS, involving Javier Garcia, John Corish, Marc Cesa, Colin Humphries

RM sent his report to the bureau to all committee members. Several topics were discussed based on the report of RM:

- It was decided that DC1 will write a specific letter about collaborations with other organizations in biochemistry and other fields. Example: Pierangelo Metrangolo got support from ICSU for his project.
- The royalties issue was discussed. It was agreed that Division 1 states that there needs to be some rules on this subject at IUPAC level. In previous cases even acknowledgements were not written. Trevor Letcher is an

example. AG said that when a book is negotiated the whole issue of royalties is ignored. In some cases the money went to the IUPAC general funds and not to the division committee. There are no royalties on the green book but IUPAC owns the copyright. In case of project books, however, IUPAC does not own the copyright. AKW will send an example of the ACS contract.

- The mix of topics in the new CPCDS committee is not appropriate (publications and chemoinformatics). The word chemoinformatics should be removed because it is used in the wrong way. Division 1 says that it should be changed.
- A discussion of the gold book took place. It was mentioned that the gold book is outdated. There needs to be a clear concept of how it should look like in the future and who is maintaining it. We need someone to be a member of the gold book committee – to go over the entries and suggest modifications. Ron Weir and Bonnie Lawlor will chair the committee. It was said that people are not aware of the gold book and they go for Wikipedia. It is important to make the gold book known. It must be updated. There are no references to PAC beyond 2008. Google search does not refer to the gold book and so does Wikipedia. We should make the gold book the official definition and Wikipedia etc. refer to this. It should be the first entry in google when searching. AF volunteered to be part of the committee. An email in this regard was sent to Bonnie Lawlor.
- DC 1 states that an option to search by project number should be added to the website
- Current website problems were discussed. Since Torino 2007 the website is discussed but even now there is nobody taking care of the website full-time. Paul Leclair does it now together with professional consultants. It was suggested that we could rather use graduate students to maintain the website. In any case there should be high priority for maintaining the website. There is a task force shared by Bonnie to work on this. It includes also Chris Brett and other people We should wait for a survey and they will collect suggestions. The members are urged to reply to the questionnaire about the website.

## **6. Progress reports on projects (AF):**

Before reporting on the progress of the specific projects, some general issues were raised:

- We should invite the project leaders present at the GA to present the projects to the division (short presentation). Maybe also in the congress. This way we can get them to the GA.

- When asking for a report about old projects we may state that if there will be no reply, there is a risk that the project will be terminated. The VP can be in charge of giving advance notice about potential termination of project.
- We should tell new project leaders to acknowledge IUPAC including the project number in publications and presentations. This should be added to the form. Otherwise it will not be considered as project output. This issue should be sent to the central office.

### **List of projects and their status:**

- 2000-026-1-100 Marsh - should be marked as terminated.
- 2001-015-1-100 Stanbury – the report by Stanbury from 10/5/2014 is " Today I submitted the manuscript of our IUPAC report on inorganic radicals for publication in PAC via ManuscriptCentral. The report is "Standard Electrode Potentials Involving Radicals in Aqueous Solution: Inorganic Radicals". It is a 258-page MSWord document, too many years in the making. A pdf of the submitted manuscript is attached. Earlier this year we also published a brief account of this report as the following: D. A. Armstrong, R. E. Huie, S. Lymar, W. H. Koppenol, G. Merenyi, P. Neta, D. M. Stanbury, S. Steenzen, P. Wardman, Bioinorg. React. Mech. 9, 59-61 (2013). A pdf of this publication is also attached. Remaining for our Task Group is to receive the reviewer comments on the Inorganic Radical report, make the necessary corrections, and publish it. We will also be generating an initial version of the manuscript on Organic Radicals shortly."
- 2001-028-1-100 Stoynov – RM emailed Chris Brett asking whether the paper mentioned in the website was published and for any new information, mentioning that if no information will be provided in two months then the project will be considered terminated.  
**Update:** since no information was obtained, this project was officially terminated on October 2014.
- 2004-036-1-100 Majer – Same story as two years ago – no response from the project leaders. The project is terminated.
- 2006-050-3-100 McQuillan –A no cost extension until the GA in 2015 was requested. A progress report will be sent until the end of June 2014. The project is likely to be concluded in the next few months.
- 2007-032-1-100 Marquadt – abridged version – is likely to finish by the end of the year.
- 2007-055-2-100 Yamanouchi – items are collected and the technical report needs to be written. A no cost extension is asked for in order to write the technical report until the GA in Korea (around 30 pages).
- 2008-006-3-100 Sun – The project is reported to be complete and the team sent a 14-page summary. We asked to modify the IUPAC website and include the new papers. The list to Fabyenne and the website updated. Then the project should be marked as complete.

- 2008-037-2-300 Griesbeck – this is a joint project with division 3. RM will be in touch with division 3 about this project and tell them that we would like to have it completed or terminated. The project is currently assigned to Div.1 on the website but this should be changed. AW sent an email to Fabyenne in this regard. Div. 3 president will contact the task group leader.  
**Update** from June 9<sup>th</sup>, 2014: Prof. Griesback sent an updated report, in which he apologizes for the delay and promises to push the project forward in the coming 5-6 months.
- 2010-009-1-100 Thommes: The project is ongoing. A final report on the project in form of an oral presentation was given at the Characterization of Porous Solids (COPS) symposium in Granada, Spain (this is one of the major conferences in the field; <http://www.cops10.org/scientific-prog.html>).
- 2010-048-3-100 Cooke – The project is progressing well. A no cost extension is requested until the end of the year. Then we will ask for a report and take it further.
- 2011-022-2-100 Tennyson – AC, who is part of the team, reported about the project. There is a recommended line shape form. The revised version was submitted to PAC at the end of April 2014 as a technical report. There will be a meeting where the participants will meet and finalize things. The project achieved its goal and will be finished upon publication. AC will ask Fabyenne to move some refs to the old project.
- 2011-037-2-100 Chirico – No response from the project leader before the meeting. AG, who is a part of the team, did not have any info. He contacted him again and this is the response send on June 2<sup>nd</sup>, 2014: "The binary system version of our Web Thermo Tables is scheduled for release at the end of this fiscal year. At that point, we will have a large collection of critically evaluated phase equilibrium data (SLE, VLE, LLE) for binary systems. We will be able to mine this collection in terms of uncertainty/chemical system type/T, p, x, y variable range/method type, etc. The data mining will be straightforward and will require no more than a couple of weeks. Preliminary results for review by the committee members should be available by the end of the calendar year. The Pure & Appl Chem article will be completed in the spring."
- 2011-049-1-100 Wallington – the project is complete.
- 2011-51-1-100 Wakeham – This project is complete – it was successful with publications. A follow up project started in 2013.
- 2012-38-1-100 Letcher – the manuscript will be delivered to the publisher by the end of June 2014 and publication is expected at November 2014. Division committee 1 should look at the final text and approve. AG will ask for it. We should also ask the publisher not to change anything. RM is in contact with Prof. Letcher in this regard.
- 2012-040-1-100 Perkins – the project progresses well and a paper was submitted. They will meet again in 2015. No cost extension until the end of 2015 is allowed.

- 2012-041-1-100 Letcher – future energy - was published in 2014. ICTNS approved it but there are still mistakes. AG will send it and RM will check and maybe an erratum will be published. We were not informed that the project is complete. RM will check who authorized completion. In the future we must insist on royalties with book projects.
- 2012-044-1-100 Metrangolo – crystal engineering – they applied for extra funding from other sources and organize their next meeting. 30K USD will be added to the budget. The project is ongoing.
- 2012-051-1-100 Goodwin – measurements were made with more to go. The project is ongoing and progressing well. It is expected to finish within a year.
- 2013-003-3-100 Wakeham – This is a continuation project and good progress is reported. It should be published a year from now. 6% royalties to IUPAC were agreed on the previous one and they asked RSC publishing that all books will be treated the same.
- 2013-035-1-100 Wallington – The project is ongoing.
- 2013-048-1-100 Stohner – the mol project - the kick off meeting is planned to the end of July. Preliminary talks were already made. JS will send a summary.

DC 1 took notice of the complaint of JP Grolier about the termination of his project 2007-002-1-100.

## 7. Finances (RM):

RM presented the financial status of the division. We received 59,200 USD for two years. 70% should be spent on projects and 30% on operations (travel). No money was spent on operations so far. Regarding projects - around 9000 USD were provided to Wallington and about 5000 USD provided for other projects (not in yet). We spent 14000 and the rest remains for the next 18 months. 15000 will be spent on the off year meeting.

## 8. New projects and future strategy:

Several new projects ideas were presented and discussed:

- a. AG: a new project about transport properties, focusing on diffusion coefficients. The project proposes updating the green book regarding definitions of diffusion coefficients. 6K USD are required. The outcome will be a recommendation in PAC and an update of the green book. Project number is 2014-010-1 and Wakeham is the project leader. This project is currently under review and more reviewers will be invited.  
**Update** from July 10<sup>th</sup>, 2014: the project was approved.
- b. AF and KB : "Guidelines for the quantitative measurement of binding affinities of proteins for their ligands" – The outcome will be a technical report and website. Funding will be requested for two

meetings, the amount depending on the location of the team members (5K-10K). The composition of the team will be finalized soon.

- c. AC: "Chemical kinetics of gas-phase elementary reactions at high temperature". The aim is to digitalize the data and evaluate rate coefficients in high temperature gas phase kinetics. The outcome will be a J Phys Chem ref data article and depositing in a database. The leader will be Tamas Turanyi. Funds will be probably around 10K.

It was decided that the three proposals will be submitted and sent out for review. Then a decision will be made by the division president in consultation with the committee members. KY mentioned that if no budget is left and we get good projects we can ask the project committee for more money.

RM received three more project proposals from Fabyenne:

- d. A proposal by Prohaska entitled "web-based platform for SNIF diagrams for selected elements". 2014-016-1. Division 2 will lead and it is related to natural isotopic fractionation. RM will ask that we will be involved in the review.
- e. Evans – 2014-018-1. The leading IUPAC body will be COCI. The proposal is VOC – Voice of the Customers data gathering. The aim is to improve the dialog between IUPAC and the companies. RM will review it and send it also to AG. We do not need to participate in the funding.
- f. Ohrstrom - 2014-001-2. This project is led by division II and our division gives 1000 USD. The topic is terminology guidelines and database issues for topology representations in coordination networks, metal-organic frameworks and other crystalline materials.

Other new projects that involve DC 1:

- g. 2013-044-1 - "preparation of the 4<sup>th</sup> revised printing of the green book, 3<sup>rd</sup> edition". JS will submit again the project for division 1.1 meeting. RM will apply for money from the project committee for commission 1.1 to meet.
- h. Division I agreed last year to support the following project 2013-037-1-200 "Creating Educational Website for Materials Chemistry". Christopher Ober from Cornell is the lead. This project is funded by Division I (\$1,000), Division II (\$1,000), and Division IV (\$1,000), and the Project Committee (\$3,000). Basically, the project aims at providing web-based education resources for young chemists in Materials Chemistry, and offering chemists in the developing world access to education tools and information. The goal is to develop a web site similar to that created by the Polymer Division.



- i. 2013-042-1 FSC project of Hernandez – division 1 endorsed but not committed to pay anything. The project committee funds it.

### **Future strategy:**

Several topics were defined in the Istanbul meeting as important for the future projects of DC1. The progress was discussed:

-Biophysics (done by AF and KB).

-Light absorption intensity (RM will not continue since there are more important new projects – will get back to it later).

-Data standardization – The projects described by AG are in this direction.

-Materials: 2013-037-1-200 is in this direction

-Shale gas: understanding the chemistry used and why and the shale gas itself "shale gas: clarifying myths and truths". Real quantitative data about the dangers and benefits should be collected. Focus on physical chemical methods to get new info and assist decision making. We will look out for potential people who can propose projects in this direction (shale gas and fluids) (RM and AG).

-DFT: a survey of methods and their pros and cons in DFT. RM and AW said that people in the field are interested. Russell Boyd is a potential task group leader (RM spoke with him). The outcome will be a glossary. A list of functionals that exist today should be made.

### **9. The international year of light (RM):**

Ideas how the division should participate are requested in 2 months until the end of July. IUPAC is not a participating member. Ideas raised are the use of light to control chemical reactions and the contribution of Bunzen.

It was decided that the cartoon competition should be in the theme of light and its interaction with matter. We will contact AR who will lead it. AF and KB will help. AF will email Andrea. Division members should contact their societies in this regard and draw their attention and report to RM and AF. AR should ask Jim McQuillan to help. We should contact the IUPAC bureau and tell them how we participate in the event. We should check what the other participating bodies are doing – FV will do it.

### **10. Sharing of committee tasks (RM):**

RM reviewed the document prepared by Jim McQuillan a few years ago. He will send the document and ask for comments until next meeting. RM will ask the vice president to share some of the work when required, for example evaluation of new project proposals.

- The role of liaison to other divisions will be added:

Jurgen Stohner – division 2

Kristin Bartik – division 3

Kaoru Yamanouchi – division 4

Anthony Goodwin – division 5

Taufiq Yap Yun Hin – division 6, representative in ChemRAWN.

Frank van Veggel – division 7

Angela Wilson – division 8

- Frank van Veggel was also appointed as a web responsible that will collect all mistakes found and report directly to IUPAC secretariat. The web responsible will have to go over the division 1 website and check it regularly.

- AF was appointed as a newsletter responsible. The newsletter can be sent to CI.

### **11. Miscellanea:**

- Replicate publications in PAC: The previous PAC editor complains that material published in PAC was replica of other publications. Specific reference is to the Rossini lecture. JS said that if both journals (PAC and the journal of chemical thermodynamics) allow it and it is clearly labeled as a duplicate just to promote it there is no problem. AG suggested that an editorial in PAC will be published instead of the replica. The question of open access was also raised. A discussion was made with arguments for and against it. AG will bring more info to the next meeting.
- Possible modifications of the division aims – delayed to next meeting.
- Suggestion to change in the bylaws: JS suggested being less strict and adding flexibility regarding the time limits for membership in IUPAC committees. AF said that the biennium period is too short. This is an item for next meeting – how to change the bylaws in this regard.

12. **Elections for the next biennium:** KY presented the topic and said we need to select the division officers for the biennium 2016-17. The suggestion is that RM will become past president, AW will become president, AF will remain secretary, Kristin Bartik is proposed as vice president. This was approved unanimously.

Taufiq Yap Yun Hin and Frank van veggel will stay as TMs for the next biennium. Four TMs (AG, AR, KY, JS) will finish their term and elections should be organized. There is no timeline yet. Five nominating committee members should be selected: two from inside and three from outside the division. KY will form the committee by the end of June and send the information to RM. KY described the election process for TMs. Voting will be in October and results in November. AMs and NRs will be elected later. This should be done by April 2015 and approved in the bureau meeting.

The chair of commission 1.1 also needs to be elected since he is a TM of division 1. We need to elect three more. We will need to be informed of the decisions of commission 1.1.

**13. 48th GA (Aug. 6-13) and 45th Congress (Aug. 9-14), 2015 Korea:**

There will be a BPC symposium in the IUPAC congress. Need some suggestions for speakers. Mainly female and people from Africa and South America. DC 1 will have a full 2-day meeting on the 5-6.8. The GA starts on Thursday 6.8.15. We can meet one day before because then we would have more time to go to other committees. We should arrive to Korea on the 4.8. RM will check if it is possible and let the others know.

**14. 49th GA and 46th Congress in Brazil, 2017:**

RM asks that the division will be highly involved in the symposium in Brazil. RM will contact people and say that we would like to be involved.