

IUPAC Division I Committee

Minutes of the IUPAC 2011 Meeting

The 2011 meeting was held at the Sheraton Hotel in San Juan, Puerto Rico from July 29 to July 30, 2011.

Present: Jim McQuillan (President)
Michel Rossi (Past President)
Kaoru Yamanouchi (Vice President)
Roberto Marquardt (Secretary) – Present on July 30, 2011
Angela Wilson (TM)
Brian Sykes (TM)
John Dymond (TM)
Rolando Guidelli (TM)

Guests: Robert Hinde (from Commission I.1)
Anatoly Kolomeisky (Young Observer, U.S. - present on July 29)
Maria Quintana (Young Observer, Peru)
James Bull (PAC Editor – visit on July 29)
Peter Mahaffy (CCE, Chair – visit on July 29)
Michael Dröscher and Colin Humphris (COCI – visit on July 29)
Kazuyuki Tatsumi (IUPAC, Vice President – visit on July 29)
John Corish (IUPAC Treasurer – visit on July 30)

1. Introduction, welcome, and apologies

The President welcomed the committee members. He conveyed apologies from Roberto Marquardt (TM, Apologies for July 29), Kristin Bartik (new TM elected), Assaf Friedler (TM), Andrea Russell (new TM elected), and Alvaro Mombrú (new AM elected). Members introduced themselves and the President closed the introduction by highlighting a number of activities taking place during the IUPAC General Assembly, and mentioned that there would be a new IUPAC website. Chris Ober, Division IV, is helping with revising of the IUPAC website.

There was significant concern as to why confirmation of elected candidates of Division I TM elections were delayed by the Secretary General as the Division had met the deadline for turning in candidates for positions. *(The supposed rationale for this was that some of the Divisions had not turned in their lists, so the entire process was delayed.)*

Elected TM (who are currently AM) should be encouraged to come to the meetings, particularly if TM are not able to attend. IUPAC has up to 10 TM positions per Division to support for travel, so the Division President should encourage these other participants if not all TM are able to attend.

2. Agenda

The following modified agenda was approved:

- 1 - Introduction and apologies (AJM)
- 2 - Approval of Agenda (AJM)
- 3 - Approval of the Minutes of Previous Meetings
- 4 - Finances (AJM/RM)
- 5 - Future Projects (AJM)
- 6 - Report to Council for the Biennium 2010-11 (AJM)
- 7 - International Year of Chemistry Divisional Activities (AJM)
- 8 - Chemical Education Committee
- 9 - Discussion of sharing of Committee Tasks/Responsibilities. (AJM)
- 10 - Elections (MJR)
- 11 - Inter-divisional Activity (AJM)
- 12 - Progress Reports on Current Projects and from Project Monitors (AJM/RM)
- 13 - Division I representatives to other Committees, Commissions, Organisations
- 14 - Advisory Committee List (AJM)
- 15 – Next meetings
- 16 - Any Other Business

3. Minutes of past meetings.

The President recapped what was discussed at the last meeting. The minutes of the Division meeting held at Hotel Krone, Zurich, Switzerland, on June 19-20, 2010 were unanimously approved.

4. Finances

The total biennium budget for Division I is \$67,300 (USD). Currently, \$11,437 has been spent for operations (17.0% of the budget) and \$21,000 in project commitments have been made, for a total of \$32,437. 48.2% of the budget has been spent. The guideline for the operations portion of the budget is no more than 30% of the budget, with 70% dedicated towards commitments.

We are committed to ~\$3,000 for the IYC competition that the Division organized. As well, \$1K was committed to an IUPAC Congress symposium speaker.

At this point, there are four project commitments:

2010-009-1-100, Matthias Thommes – Physisorption of gases, with special reference to the evaluation of surface area and pore size distribution. Commitment \$5,000. Total commitment \$5,000.

2008-037-2-300, Axel Griesbeck – Standard photochemical processes. Commitment \$5,000. Total commitment \$10,000.

2010-033-2-024, Bonnie Wallace – JCAMPX-CD: Standardization of data and meta-data formats for circular dichroism and synchrotron radiation circular dichroism spectroscopy, and interface with the protein circular dichroism data bank. Commitment \$6,000. Total commitment \$9,800.

2010-048-3-100, Stephen Cooke – Common values of nuclear electric quadrupole coupling terms for appropriate nuclei in functionalized hydrocarbons. Commitment \$5,000. Total commitment \$5,000.

5. Possible projects that may be forthcoming, or have just arrived.

John Dymond mentioned that there are four Thermodynamics project proposals that will be coming from Anthony Goodwin. The topics include phase equilibrium and liquid systems (pure and mixed).

A project proposal had just arrived by Professor Jonathan Tennyson. “Intensities and line shapes of water transitions from experiment and theory”. \$30,000 was requested for the project. There was some discussion of the prior progress on their efforts. Two high visibility papers have been published on this topic, and two papers are forthcoming (the work is completed). For this new project, there has been a ~50% change of personnel.

There was a discussion about how such high profile projects can bring more attention to IUPAC. Making the IUPAC support more evident in databases was discussed, as was better visibility on the website.

Further suggested areas for projects include: biophysics – i.e., metalobomics (B. Sykes; genomics, molecules of life), hydrophobicity, biomimetic membranes (R. Guidelli), protein dynamics, project on charge transfer coefficients (R. Guidelli), the preparation of an appendix to the GB abridged version that contains a variety of examples of the good use of symbols and units in physical chemistry (R. Hinde, R. Marquardt).

Roberto Marquardt recalled that the role of TM is to primarily search for colleagues who will propose adequate projects, rather than to propose projects themselves.

Maria Quintana asked about the type of IUPAC projects; she was then informed by the committee on the general form and contents of IUPAC sponsored projects and how to access the information on the IUPAC web site.

Off agenda item: Visit from Pure and Applied Chemistry Editor.

James Bull, editor of Pure and Applied Chemistry visited the meeting on July 29 at 10:00. He commended the Division for being a strong producer of high profile products. He said that they are looking for products on new, developing, and evolving fields and hot/new topics. They can do special issues/special projects. Dr. Bull said that he could work on an entire endeavor (i.e., deal with all invitations, reviews, . . .), or could do part of it or get teams involved. He has flexibility.

6. Discussion of the Division I Report to IUPAC Council for the 2010-2011 biennium

There was discussion about from where most of the division projects come. The divisional structure existing since 2000 is not generating many projects to date. For example, no projects seem to be coming from the NR-level. There seems to be a drop off in terms of the number of projects.

It was suggested that a brief overview of the projects that are going on in our Division be sent to the TM, AM, and NR. The President indicated that in June an e-mail message about the Puerto Rico meeting which included highlights of projects were sent to all TM, AM, and NR.

7. Activities in the International Year of Chemistry

The President thanked Rolando Guidelli for putting together the guidelines for the IYC poster and video competitions for the division. Assaf Friedler was also acknowledged. The winner of the cartoon competition will be acknowledged at 6:30 pm on Monday during the Congress.

The award winner was Jessica Hough, a high school student from Montgomery, New York. The Division promised a \$1,000 award. Corning also contributed \$1,000, and the American Chemical Society contributed some funds as well. There was some discussion in terms of whether or not further funding should be provided to the student. The general feeling was that the Division should not provide additional funding.

The video competition was not as popular. Videos are actually team efforts, rather than individual efforts. We had opened the competition to individuals only. It was remarked as well that two minutes were perhaps too short of a time limit on the videos. Some members were of the opinion that the length was just fine.

We called the winner of the IYC video competition winner, Yordan Darakchiev from Bulgaria, to congratulate him by Skype. Both the President of the Division and the Vice President of IUPAC congratulated the high school student on his award.

Generally, the competitions were seen as successful activities. In future actions, NAO should be activated earlier by the Secretary (through the NR). Angela Wilson said that IUPAC should send an official letter of acknowledgment to the winners of the competitions. A brief report note on CI with figures should also be provided by the President of the Division.

8. Visit of Peter Mahaffy, CCE

Peter Mahaffy has provided Roberto Marquardt with a list of biennium activities of CCE. He asked that their list of priorities be shared with others (TM, AM, NR). There have been a number of priorities of CCE over the biennium.

1. Preparation for IYC.
2. Focus on the importance of learner-centred chemistry curriculum and education
3. Connection between chemistry and sustainable development.
4. Build chemistry education networks.
5. Take the international conferences on chemical education (ICCE) that include ~300-600 people with other activities in Rome, July 2012.
6. Ethical issues in chemistry.

For IYC, some of the activities that were highlighted were the development of an interactive periodic table (isotope focus), the worldwide water experiment (so far, over 10,000 people have participated).

Peter suggested that we contact him if the Division has ideas about possible activities for or interactions with CCE.

There were some brief comments about a possible tie that Peter encouraged the Division to examine. See, explainingclimatechange.com – Lesson 4.

9. Discussion on Division I committee tasks

The President provided a document with suggestions about the roles and responsibilities of members of the committee. There was some discussion, and the President encouraged the Vice-President to use this for possible guidance in the future.

It was noted that there is now a two-year , rather than a four-year appointment for TM.

Off agenda item: Visit of Michael Dröscher and Colin Humphris, COCI

Michael spoke with the Division about partnerships with industry. He mentioned COCI interest in tools for international standardization via a proposed project on life cycle analysis (from cradle to cradle (*not from cradle to grave*)). He mentioned assisting chemistry-related industry with regard to sustainable development and growth. Some activities in this area were in international chemicals management, responsible care, and an industrial prize for sustainability.

COCI is working with CCE on the public appreciation of chemistry.

Colin Humphris discussed the World Chemistry Meeting that will be held next week. He said that the program will go live on the internet on August 16. He mentioned that an earlier meeting of this sort on women in chemistry held in May had 27,000 participants.

10. Report on nominations.

Michel Rossi discussed the 2012-2013 membership panel. A five-member nomination committee involving two members (Michel Rossi and Assaf Friedler) of the Division and three external persons (Chris Brett, Ron Weir, and Z.-Q. Tian) selected candidates. Michel suggested that in the future, potential candidates should be contacted by phone. There were eight candidates for four positions. The list of areas of particular interest identified at the off year meeting were thermodynamics, kinetics, biophysical thermodynamics, membranes, biological NMR, energy storage and conversion, nanotechnology, single molecule detection, colloidal chemistry and interfaces, and soft matter physical chemistry.

The four new elected TM are Kristin Bartik, Anthony Goodwin, Andrea Russell, and Jürgen Stohner (who is also Chair of Subcommittee I.1). The new elected AM are Attila Csaszar, Vadim Kukushkin, Vesna Miskovic-Stankovic, Alvaro Mombrú, and Xin Sheng Zhao.

11. Interdivisional activity.

Interdivisional Subcommittee on Materials Chemistry – With Michel Rossi “retiring” from the Division at the end of this biennium, there is a need for another divisional representative on this subcommittee. Angela Wilson will continue on this subcommittee. Michel Rossi, Jim McQuillan, and Angela Wilson attended the subcommittee meeting on July 28, 2011, and provided a discussion. The chair of the subcommittee, Len Interrante, organized a Materials Symposium for the IUPAC Congress which was successful in obtaining funding from the ACS.

Interdivisional Committee on Terminology, Nomenclature, and Symbols (ICTNS) - John Dymond provided a brief update on ICTNS. ICTNS has been concerned about publications that have bypassed IUPAC approval. It was suggested by John that task groups be made aware that their publications (books, in particular) be approved by IUPAC. They should not be published with the IUPAC logo without having gone through proper approval.

12. Status of current projects.

Recently, the gathering of information about project status has been the responsibility of project monitors that have been assigned by the Secretary. The President suggests that in February each year, reports need to be gathered on projects. This is very critical timing in regards to reports to the Bureau.

2000-026-1-100 (Marsh) – 100% of the budget has been spent. A couple of the primary task group members have retired. However, it is anticipated that this will be wrapped up within the next twelve months.

2001-015-1-100 (Stanbury) – When will the tasks be finished? Stanbury told Rossi that they are still waiting for results from a couple of the task members. The President will contact Stanbury.

2001-028-1-100 (Stoynov) – Stoynov hopes to complete the project this year.

2001-036-1-300 (Braslavsky) – Michel Rossi views this project as complete. Final reports have been submitted as recommendations to PAC.

2001-024-1-100 (Ruscic) – This project resulted in one publication. Michel Rossi asked for the final report on a couple of occasions, as has Jim McQuillan. Ruscic has not responded to these requests. There is ~\$3,500 remaining in the budget. The Division decided to terminate this project. The President will notify Ruscic of the termination of this project.

2003-056-2-500 (Murray) – At this stage, the task force is on their sixth resubmission of a manuscript on terms and definitions relating to mass spectrometry. They began submitting this manuscript in 2006. For IUPAC recommendations, 15 reviewers must approve.

2004-026-2-100 (Arunan) – The recommendations and technical report have appeared in Pure and Applied Chemistry. Therefore, this project has been completed.

2004-035-1-100 (Tennyson) – Task group members have told us verbally that they have published two papers on this project, with two additional publications supposedly being completed.

2004-005-2-500 (Majer/Sedlbauer) – Progresses well.

2004-005-2-500 (Camoës) – This project is complete.

2006-021-2-100 (Rouquerol) – Is almost completed, lineage received great credits. Unspent money can be used to pay photocopies and postage.

2006-023-3-100 (Alberty) – The submitted recommendation has been declined by ICTNS and was therefore not published in PAC, but in *Biophysical Chemistry*; no IUPAC funds have been spent on this project, which the committee considered therefore to be concluded, while issuing its disappointment for the efforts done both from the Division as well as from the Task Group. The President presented a letter from Dr Robert Goldberg, who explained that it turned out to be impossible to produce a set of recommendations that would be acceptable both to IUPAC and to biochemists. Clearly, more effort from the Division is necessary in order to improve the situation of this important field of activity in the future.

2006-050-3-100 (McQuillan) – This project is in progress and a no cost extension is asked.

2007-002-1-100 (Grolier) – Wait for August to see outcome of July meeting and decide then to ask for a no cost extension.

2007-024-2-100 (Chirico) – Project sent to review, internal and external simultaneously.

2007-032-1-100 (Marquardt) – Project should be finished by the end of this year; indexing and final formatting is still missing.

2007-048-2-100 (Ramasami) – There are problems with this project and the committee has taken contact with the task group chairman in order to request modifications.

2007-055-2-100 (Yamanouchi) – Almost all TG members are active, half of the manuscript is written, a no cost extension is requested.

2007-040-2-200 (Martinez) – No report is available; the project is led by Division II and the Secretary will request a report from them.

2007-010-2-500 (Bode) – No report is available; the project is led by Division V and the Secretary will request a report from them.

2007-039-1-024 (Frenkel) – Revolutionary project, major journals are using published recommendations; the manuscript, the ThermoML scheme and 14 use cases were submitted to PAC as IUPAC recommendations, subject to ICTNS review; the ThermoML scheme being very complex, the reviewing process is expected to be long.

2008-006-1-100 (Sun) – Despite large list of publications, no direct link with IUPAC project; the three components of the project (see web page) have not yet been addressed, but there is still sufficient time to complete.

2008-045-2-200 (Assael) – This project is complete.

2009-031-2-100 (Wallington) – Snapshot of the database done (visited about 1000 times per week), first round took 10 years; second round will be next projects; project's budget is needed now to meet for performing updates of web site.

2009-032-1-100 (Metrangolo) – The project is running very well, a first meeting was held in May 2010 and a second and potentially final meeting will be held in Spain in August 2011.

2010-009-1-100 (Thommes) – Project just started; it is appreciated that the TG leader comes from industry.

2010-033-2-024 (Wallace) – Project just started, the project has been leveraged to the BBSRC.

2010-010-4 (Interrante) – The project has been declined. The Materials Chemistry sub-committee will be chaired in future by Chris Ober of Div IV who will prepare a pedagogical web site in order to address more professionals.

2010-048-1 (Cooke) – Project has just started.

A discussion took place on the format of the compilation of progress reports. A new procedure to collect reports was chosen, in which the information is recorded in a form that is simpler and clearer than formulated by the project evaluation committee: a report should have a maximal length of 10 lines, stating how much of the objectives have been reached and what the major difficulties were; reports will be requested annually around the end of January in order to be delivered by February 28; the request email should have an official format, i.e. it should include the IUPAC logo. Roberto Marquardt prepares a template spreadsheet for the compilation of all projects; that spreadsheet contains a column recalling the objectives. The possibility of handling project reports via a web page form is discussed. This format to treat progress reports shall be proposed to the projects evaluation committee.

13. Division I representatives to other bodies

The updated list of representatives is attached to these minutes.

Kaoru Yamanouchi will represent Div I in CCE on the 46th GA.

14. Advisory Board list

The President asked committee members to review the list of members of the Advisory Board and to make propositions to him as to its renewal.

15. Next meetings

The off-year meeting will probably take place in Japan around May or June 2012. The potentially high cost of the meeting was discussed and it was decided that the Division could afford this, if total costs do not exceed the 30% budget limit. Kaoru Yamanouchi proposed to organize a one day scientific meeting in addition to the committee meeting, which was highly welcomed. If possible, the host institution will help covering the expenses of the meeting.

Mention is made of the 47th GA in Istanbul, between August 9 and 15, 2013.

16. Other business

Roberto Marquardt reported on some conflicts existing between Commissions I.1 and II.1 and complaints about the apparent lack of reaction of Commission I.1. He explained that the Commission has always answered to queries about the Green Book in reasonable time. He also reports on the potential new role of Commission I.1 as a permanent adviser to ICTNS, a role which was proposed by the Chairman of ICTNS, Prof. Ron Weir. He said that this is a new interesting proposition, that would however make necessary to enlarge Commission I.1 in order to guarantee rapid replies from specialists. Also, Commission I.1 should then be able to meet more regularly, for instance, during the General Assemblies. He recalled that Commission I.1 has no proper budget and that it depends on the Division I budget. Alternatively, Commission I.1 members may apply for short term projects in order to finance off-year meetings needed to settle controversies related to queries from ICTNS or other bodies.

Rolando Guidelli indicated concern about an electrochemical notation that is not correctly represented in the Green Book. Roberto Marquardt sent this concern to Christopher Brett. As Robert Hinde, who is a member of Commission I.1 is present at the meeting, Rolando was asked to send Robert the documentation about this issue.

It was suggested that IUPAC has a clear procedure for reporting any corrections/modifications that may be needed for the Green Book (and for other such books).

A short project out of our Division that comes to a recommendation on how to address the problem has been recommended. It was suggested that an international group of individuals develop a short technical report on the history and conclusions in order to try to advocate the change with the Green Book.

Departing members John Dymond, Brian Sykes and Michel Rossi are cordially thanked for their work and contributions to the Division.