

IUPAC Division I Committee

Minutes of the Off-Year Meeting 2010

The 2010 off-year meeting was held at Hotel Krone, Zurich, Switzerland, from June 19 to June 20, 2010.

Present: Jim McQuillan (President)
Michel Rossi (Past President)
Kaoru Yamanouchi (Vice President)
Roberto Marquardt (Secretary)
John Dymond (TM)
Assaf Friedler (TM)
Rolando Guidelli (TM)
Angela Wilson (TM)

Apologies: Jiang Guo Hou (TM)
Brian Sykes (TM)

1. Introduction, Welcome and apologies

The President welcomed the committee members. He conveyed apologies from Brian Sykes (TM) and Jiang Guo Hou (TM). Members introduced themselves and the President closed the introduction by explaining the actions to be taken for the next biennium.

2. Agenda

The agenda was approved.

3. Minutes of past meetings

John Dymond said that a practice of good policy is to remind what was decided in the last meeting. So was the procedure and the minutes of the Division meeting held at the GA in Glasgow in 2009 were approved.

4. Aims and objectives

A discussion followed on aims and objectives of Division I.

Roberto Marquardt explained the objectives of the work followed by Commission I.1, which is the sub-commission of Division I responsible for terminology, symbols and units of use in Physical Chemistry. The main aim of the work is the maintenance and update of the Green Book, which is briefly presented.

A debate followed whether it would be useful for IUPAC to keep databases for structure and spectroscopy, such as the NIST database, support for which was said to be closing.

In this context the policy of short term projects was addressed and questioned as to its efficiency with respect to database related projects. It was proposed that database projects could be retained by a series of related short term projects. Examples are given for database projects that failed, such as the ionic liquid database. Finally, it was said that the

idea of involving Division I more strongly in database projects should receive increasing attention. Lack of financial support from project funds could be compensated by collaborations with non-profit organizations.

Jim McQuillan said that the two last points of the aims and objectives have not yet been much followed. These are:

- recognize new developments in physical and biophysical chemistry and its 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.

5. Reports on current projects

120/15/95 (da Silva) The major problem related with this project is the non-conformity of the recommendation with IUPAC rules. There have been conflicting views from reviewers. It is suggested to write to the author whether the project should be abandoned.

150/24/95 (Heyns) Similar case as above mentioned, similar suggestion.

2000-026-1-100 (Marsh) 12-months no-cost extension request approved.

2001-015-1-100 (Stanbury) No action needed, a no-cost extension was granted.

2001-028-1-100 (Stoynov) ditto.

2001-036-1-300 (Braslavsky) The project is expected to be complete. The Secretary queries with Division IV.

2001-024-1-100 (Ruscic) Michel Rossi gave a detailed report on this project, the result of which should have been the publication of three volumes. Volume 1 has been published in Phys. Chem. Ref. Data in 2005. Volume 2 is 80% complete and volume 3 has not started. It is suggested that a no-cost extension be requested until the end of 2010 to grant completion of a 2 page report – not of volume 2. Michel Rossi will solicit the report. The question is raised as to a new project. Angela Wilson would address Jan Martin in this respect.

2003-036-2-100 (Corti) Successful completion.

2004-026-2-100 (Arunan) A long discussion took place with respect to technical and scientific aspects of the proposed recommendation. It is finally agreed that additional reviews are needed and five names of new reviewers have been proposed. The repetition of the recommendation must be deleted from the technical report that accompanies it.

2004-035-1-100 (Tennyson) A no-cost extension request until end 2010 is approved.

A discussion took place on the general procedure of the submission of recommendations and technical reports. It was concluded that there are clear guidelines for this procedure. It

is suggested that in Division I a parallel procedure is started by the Division President as soon as draft is posted for internal reviewing, which involves expert members of the Division (among TM, AM, NR and AC), and the Division Secretary, for information.

2004-036-1-100 (Majer/Sedbauer) A presentation of a TR draft on two conferences end 2010 is foreseen. Money should be spent in 2011 for publicity. A no-cost extension request until end 2011 is approved.

2006-021-2-100 (Rouquerol) A document is almost in final stage to go for internal review. A no-cost extension request until end 2010 is approved.

2006-023-3-100 (Alberty) Mention is made of problems related to acceptance of draft. A. Goldberg is supposed to take over the project. J. McQuillan shall write to encourage members to meet and finish project – use can be made of project budget. A no-cost extension request until end 2011 is approved.

2006-050-3-100 (McQuillan) The project has slower progress than foreseen; in particular the surface-enhanced IR turned out to be very challenging for teaching. A no-cost extension request until March 2011 is approved.

2007-002-1-100 (Grolier) A document should be ready by the end of this year. A no-cost extension request until end 2010 is approved.

2007-024-2-100 (De Loos) There are problems related to an illness of the main contributor. A no-cost extension request until the middle of 2011 is approved.

2007-032-1-100 (Marquardt) This project is lagging behind schedule; one problem is certainly a too optimistic view of the work related with an appropriate reduction of the contents of the Green Book (GB) into an abridged student's version; the publication of the abridged version of the GB for the IYC is probably out of reach. TM will inquire task group members about the project's progress.

2007-048-2-100 (Ramasami) The Technical Report is in internal review.

2007-055-2-100 (Yamanouchi) 75% of the budget has been spent for an international conference (2010 Pacific Meeting) to discuss the procedure, assignments and the home page. Submission is foreseen at the beginning of 2011.

2007-010-2-500 (Bode) No further information available, the secretary will write to Div V to inquire. A no-cost extension should be requested.

2007-039-1-024 (Frenkel) J. Dymond has been assigned to this project and will report on it at the next meeting. A no-cost extension is requested until end 2011.

2007-050-2-600 (Letcher) This project is complete. However, a discussion took place on the general policy regarding book projects, in particular the review procedure for books. The Secretary General should draft a letter informing about the contract or a provisional information on the contract contingent upon transfer sponsoring from the Division in order to insure the quality control of contents. It seems that ICTNS has been informed by John

Jost in certain cases. The question on royalties has also come up and the Division should be aware of the policy.

2008-006-1-100 (Sun) The project is progressing well.

2008-014-1-100 (Sengers) The document is in production, the project is complete.

2008-045-2-100 (Assael) The project is complete.

2008-039-2-600 (Letcher) This project is complete, the book "Handbook on Waste Management and Recycling" will be available in 2011 (for about 95 USD). There has been no final report to Div I.

2009-031-1-100 (Wallington) A meeting took place on June 12 and 13, 2010; there have been publications in Atmospheric Chemistry and Physics; the maintenance of the web site database is secured by other sponsors. The project shows good progress.

2009-032-1-100 (Metrangolo) A first workshop with a meeting of the task group took place on May 7; a second workshop is foreseen in July 2011. The project shows good progress.

2010-009-1-100 (Thommes) The project just started.

The following three projects are currently under review:

2008-037-2 (Griesbeck) In revision.

2010-010-4 (Interrante) In a discussion, the great need for standardization is recalled. IUPAC should play a bigger role in what is related to chemistry within material science. The meeting foreseen in Boston will allow to reformulate the proposal. The focus should be on materials, rather than material sciences.

2010-033-2 (Wallace) In revision; is the term "meta-data" well defined? A. Friedler will become monitor of this project.

Following the discussion on projects 2007-050-2-600 and 2008-039-2-600, Div I will check with the secretary general to see whether task group chairs are well informed about the proper procedure for projects that also involve the publication of books. It is also stated that AM, NR and members from the advisory board should be more involved in the revision process, in particular of books.

6. Finances

The total biennium budget for Div I amounts to 67300 USD. Currently, 4864 USD and 5000 USD have been spent for operations (7.2% of the budget) and project commitments, respectively. It is recalled that the guideline for operations is 30% of the budget, with 70%

for commitments.

7. Future strategy and new projects

Future strategies will focus on the development of biophysical chemistry (see point 8 below).

Beside this main stream line, other projects should be continued. It was reminded that A. Wilson proposed some time ago a project related to theoretical and experimental spectroscopy of heavy elements. This project has been rejected but it should be reformulated and resubmitted.

Another project could be related to a web site project on databases for molecular structure and spectroscopy, similar to the CCCBD data base currently maintained by NIST.

Projects related to the IYC 2011 are addressed below.

8. Discussion on steps to strengthen the role of biophysical chemistry

A. Friedler explains that biology is split into several divisions and so it is difficult to talk on a single role of biophysical chemistry. He raised the question whether there should not be a subcommittee on biophysical chemistry that would include all different divisions of biology. He saw a need in convincing people to collaborate. A. Friedler sees the measurement of binding affinities in protein-protein interactions as a main emerging topic worth to be proposed as a project. Activities would range from database to methodology assessments.

R. Guidelli puts the focus on the role of functions. He says there is a gap to be bridged between known solid state NMR studies and environmentally dependent situations. A database is needed on redox potentials of proteins and related methods. He finally asks "what kind of measurements can be performed to learn more about membrane physics?"

K. Yamanouchi knows a membrane dynamicist in Heidelberg; who writes to him to ask about running an IUPAC related project?

9. Elections for the next biennium

The Past President explains the procedure for the selection and election committee. Two internal and three external members are suggested for the election committee: R. Guidelli and A. Friedler, R. Weir, W. Baumeister and Z.-Q. Tian. Electorate should include advisory board and task group chairs.

R. Marquardt agrees to become Vice President and A. Wilson agrees to become Secretary in the next biennium.

R. Marquardt will finish service as Chair of I.1 and he proposes J. Stohner to become new

Chair of I.1.

Currently the following areas of physical chemistry will have continuous representation in Div I:

surfaces, interfaces (J. McQuillan)
gas phase spectroscopy, reactions (K. Yamanouchi)
quantum chemistry, quantum dynamics, spectroscopy (R. Marquardt)
protein interactions, biophysical chemistry (A. Friedler)
electrochemistry, biophysical chemistry (R. Guidelli)
quantum chemistry (A. Wilson)

Missing areas are the following (names for potential new members are given in parentheses):

thermodynamics (Goodwin)
kinetics (J. Stohner)
biophysical thermodynamics, membranes, biological NMR (K. Bartik)
energy storage and conversion
nanotechnology, single molecule detection
colloidal chemistry and interfaces
soft matter physical chemistry

The advisory board is not well distributed. TM are asked to think of new suggestions and deletions.

10. Division I representatives on other bodies

A list is prepared and attached to these minutes.

11. Interdivisional activities, including Materials Chemistry

A discussion on materials chemistry was carried out under point 5 above.

The main topic related to interdivisional activities involve the IYC 2011 (international year of chemistry 2011).

Apart the ideas shared during the Division I meeting in Glasgow, several additional ideas were evoked. J. McQuillan comes up with the general idea of using simulations or modeling. M. Rossi evokes videos currently available on the web that make chemistry popular and gives the example from www.periodicvideos.com. R. Marquardt recalls the pedagogical videos from Anna Krylov.

Finally, an idea was retained that consists of proposing a contest among school kids on the best video to illustrate a physical chemical process. Tool kits to construct a video on the

internet should be make available and division funds as well as grants from IUPAC task group on the IYC 2011 project should be used for that. Alternatively to a video, and much simpler to implement, a second contest should be launched asking for the best cartoon or comic that illustrates a physical chemical process. The prize could be a grant to come to the 2011 IUPAC World Congress, or alternatively stimulating trip to a renowned scientific location such as NASA, CERN, etc..

12. 46th General Assembly in Puerto Rico, 2011

The following meeting dates are fixed: Friday, July 29 and Saturday, July 30, 2011 in Puerto Rico.

13. 47th General Assembly in Turkey, mid August 2013

Mentioned.

14. Any other business

A discussion is started on the definition of roles that TM, AM , NR and members of the advisory board to Div I should take. J. McQuillan will send a draft proposal containing some ideas in the near future.