

Summary minutes of meetings of the Physical Chemistry Division Committee during the 39th General Assembly of IUPAC, Geneva, 23–27 August 1997

The future structure of IUPAC and the reorganization of the union that is expected as a result of the work of the Strategy Development and Implementation Committee were extensively discussed during the PCD Committee meetings. It was generally felt that changes are needed. The organization is elaborate and inflexible, and the work should be more focused on subjects which are coordinated over an international scale. The present statutes of IUPAC are too vague and nonspecific to allow the measurement of achievements. Its activities can be considered to represent two different interest areas: a scientific side exemplified by the 'Green Book', and

data compilation and bodies such as CHEMRAWN and COCI on the other side. It was generally felt that the suggestions for restructuring in the VPCA report, involving the mergers of Commissions of the Analytical and Physical Chemistry Divisions would not result in a more responsive or relevant organization. Divisions and Commissions are criticised for not fulfilling the IUPAC mission, yet this mission remains vaguely defined.

To set the stage for the discussion, each participant of the meeting was asked to answer the question 'Would IUPAC be created if it did not exist?' There was a consensus that an international body is needed for matters such as international nomenclature, atomic weights, tables of thermodynamic and thermophysical properties

of substances of great commercial interest, etc. Such a body is also needed for sorting out units, and to formulate guidelines for presentation and codification in rapidly moving and newly developing fields. It could also act as a pressure group on governments in special issues. This body could be much smaller than the present IUPAC and more flexible, with a short response time. The discussion was centred on the question of what changes are needed in the Physical Chemistry Division in the next 2–4 years. The question was raised, 'What would happen if most or all permanent commissions were abolished?' After some discussion, the Commission Chairmen decided to meet as a group to discuss this question. In the interest of making the Physical Chemistry Division more flexible and relevant they recommended the following:

- 1 The Commission Chairmen should become a permanent part of the Division Committee which would otherwise be reduced to a few officers and an at-large TM.
- 2 At least an entire day of each General Assembly meeting should be devoted to discussions of scientific and technological issues as possible candidates for IUPAC projects. This discussion would involve the newly constituted Division Committee. Discussion of administrative issues would not be permitted during this period. Ideas would be circulated in advance of the GA, giving members of the Division Committee time to get input from scientific colleagues outside IUPAC.
- 3 Such discussions would lead to new projects, perhaps involving members of several Commissions. The Commissions would interpret their missions broadly and this, in time, will lead to appropriate changes in the Commission structure. Coordination with other Divisions would also be possible.
- 4 The need to keep the Commission structure was emphasized by the comment, 'Abolish the Commissions and IUPAC will die because of lack of projects'.

The Division Committee approved these recommendations and decided to propose to the IUPAC authorities that the membership of the Physical Chemistry Division Committee be changed to Commission Chairmen, a few officers and a position for a titular member from outside the existing Commissions.

Gerd Olofsson

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Quantities, Units and Symbols in Physical Chemistry. Commission on Physico-Chemical Symbols Terminology and Units (I.1) at the IUPAC General

**Assembly 1995, Guildford, UK,
4–7 August 1995**

**Summary minutes prepared by Martin Quack,
Secretary I.1**

The Swedish translation of the abbreviated list of Physical Chemical Symbols has just been published and a German translation of the green book is underway. There seems to be a need for a better coordination of the translations. Further possible translations (into French, Italian, etc.) were discussed.

The versions of the green book for the 3rd edition, with the new title *Physical–Chemical Quantities, Units and Symbols*, which is planned for 1998, were discussed in detail. Of the numerous topics, we shall mention here only the more general issues which remained unresolved and still need further discussion. The question of the definition of the 'Electrochemical Potential' has been discussed and it was decided that a small subcommittee of five people, formed by some members of I.1 and I.3 (Electrochemistry) should prepare a definitive formulation which is acceptable to both I.1 and I.3 until the next meeting.

The central term 'amount of substance' remains controversial because of its clumsiness. Possible alternatives were discussed, with the idea of introducing a clearly technical term, which is not taken from the English language, such as 'enplethy' (from Greek, similar to enthalpy, energy, entropy), 'Stoffmenge' (from German) 'Stoffamount' mixed (German and English) and 'ment'.

In a meeting with I.5 (Spectroscopy) the introduction of an SI consistent unit for the quantity wavenumber (rarely called also 'repetancy') was discussed. One proposal is 1 Berg = 1 Bg = 1 m⁻¹ (in analogy to 1 Hz = 1 Hertz = 1 s⁻¹). The frequently used unit 1 cm⁻¹ would be replaced by 1 hBg (hectoberg), which is SI consistent and easily pronounced.

**Meeting of the Commission on Biophysical Chemistry (I.7), Geneva, Switzerland,
24–25 August 1997**

Helmut Hauser, as the Commission Chairman, first gave an overview of the directions that IUPAC was being urged to take. A more restrictive policy in selecting IUPAC projects will be adopted. Future IUPAC projects should be timely, highly relevant to the chemical community and completed in a reasonable period of time.

The main items on the agenda were the review of ongoing projects and the discussion of feasibility studies. The project 'Recommendations for the Presentation of NMR Structures of Proteins and Nucleic Acids' coordinated by Kurt Wüthrich has been completed and is scheduled for publication in *Pure and Applied Chemistry* by the end of 1997. The plan is to also have it pub-

lished in the *Journal of Molecular Biology*, the *European Journal of Biochemistry*, *Biochemistry* and the *Journal of Biomolecular NMR*. There was a general consensus among the members of Commission I.7 and the Division Committee that this document represents an important contribution by IUPAC. It will prove very valuable in the standardization of the reporting of NMR structures of proteins and nucleic acids.

In a joint meeting with the Electroanalytical Chemistry Commission V.5 (R.P. Buck, Chairman) Daniel Thévenot's project on Electrochemical Biosensors was reviewed. A 'final' document has been sent to eight journal editors, about 20 experts and the members of the two commissions involved. It has already been approved by the Interdivisional Committee on Nomenclature and Symbols (IDCNS). The present definition of biosensors excludes 'single use devices'. This fact has turned into a contentious issue that needs to be resolved satisfactorily in the final document. The completion date of this project is 1998.

Robert Goldberg's project on 'Thermodynamics of Enzyme-Catalyzed Reactions' was discussed in a joint meeting with the Thermodynamics Commission I.2 (W. Wakeham, Chairman). This project, which is now formally complete, has led to three publications in the *Journal of Physical and Chemical Reference Data*:

- R.N. Goldberg & Y.B. Tewari. Thermodynamics of enzyme-catalyzed reactions: Part 3. Hydrolases. *J. Phys. Chem. Ref. Data* 1994, **23**, 1035–1103.
- R.N. Goldberg & Y.B. Tewari. Thermodynamics of enzyme-catalyzed reactions: Part 4. Lyases. *J. Phys. Chem. Ref. Data* 1995, **24**, 1669–1698.
- R.N. Goldberg & Y.B. Tewari. Thermodynamics of enzyme-catalyzed reactions: Part 5. Isomerases and Ligases. *J. Phys. Chem. Ref. Data* 1995, **24**, 1765–1801.

Robert Goldberg pointed out that the database needs updating as new information appears in the literature. There is now a need and an opportunity to derive Gibbs free energies and enthalpies of formation for biochemical substances from thermodynamic network calculations.

Hans-Jürgen Hinz and Fred Schwarz presented the third draft of a document dealing with 'Recommendations for the Measurement and for the Presentation of Results Obtained on Biological Substances with Scanning Calorimetry'. The scope of the final document was discussed in detail. To finalize the project in 1999 the working party will meet twice within the next year.

Martin Caffrey reported on the status of the project on 'Nomenclature for Lipid Mesophases'. He summarized the objectives of the project and described his strategy for realizing these objectives. A first version of a document entitled 'Recommendations for a Lipid Phase No-

menclature' has been drafted by the working party and this will serve as a basis for the preparation of the final document. The expected completion date is 1999.

Helmut Hauser reported on the status of the project 'Terminology in the Field of Lipid Vesicles'. The recent expansion and numerous new developments in this field of research called for an updating of the existing document written by Lisbeth Ter-Minassian-Saraga. For this purpose a new working party has been formed and an amended version of the document is due within the next year. The expected completion date is end of 1998.

In a joint meeting with the Electrochemistry Commission (I.3), Fred Hawkridge and George Wilson reported on the status of the joint project 'Redox Potential Measurements of Proteins'. Current plans include making the report consistent with the IUPAC Green Book, collecting and incorporating the comments of various expert reviewers, and producing a final version to be sent to IDCNS for approval in 1998.

Terry Stouch presented his feasibility study on 'Recommendations for Reporting the Results of Computations in Biophysical Chemistry'. Stouch has established a well-balanced working party of experts who concluded unanimously that there is a need for guidelines for the presentation of computational results. All members of the Commission agreed that this subject is of great importance to science and that it warrants the initiation of a new IUPAC project. It is conceived as a joint project with Professor J.E. Boggs of the subcommittee on Theoretical Chemistry of Commission I.5.

The time left was used for discussion of possible future projects that might be undertaken within Commission I.7 or as joint projects with other commissions. In several joint meetings with Commissions of the Physical Chemistry Division and also other Divisions the need for good coordination and collaboration within IUPAC was emphasized. John Ralston, Chairman of Commission I.6, stressed that making use of existing expertise within IUPAC by optimizing coordination and collaboration is preferable to generating new IUPAC bodies.

**Dr John R. Moody, Chairman, acting for the vacant position of Secretary*

Minutes of the 6th Meeting of the Commission on Isotope Specific Measurements as References (II.4), University of Geneva, Geneva, Switzerland, 27 August 1997

Present:

Dr John R. Moody (Chairman)

Prof. Kensaku Okamoto

Dr John W. Gramlich

Dr Andréé Lamberty

Prof. Kevin J.R. Rosman
Dr Philip Taylor
Dr Robert Vocke
Prof. Paul De Bièvre
Prof. Klaus G. Heumann

Apologies for absence: Prof. Robert F.M. Herber
'The International Measurement Evaluation Programmes (IMEPs) for rounds 1–6 have been completed, with the exception of several publications that are in press or prepared for review. The concept of comparing the 'state of the practice' to a reference value established by isotope specific measurements traceable to the SI have been well received by programme participants and by IUPAC. The practice is likely to spread through the development of numerous regional IMEP programmes initiated by Prof. De Bièvre, thus multiplying the influence of the Commission programmes.'

Summary

The members were welcomed to the meeting by Dr J.R. Moody. The minutes of the 4th Meeting of the Commission II.4 in Guildford, UK on 6–7 August 1995, were adopted as distributed. The agenda of the 6th meeting was adopted without amendments. New officers were elected with Prof. K. Okamoto assuming the position of Chairman. Dr J. Moody will continue service for two more years as Secretary in order to assure a smooth transition. Prof. Z. Motion of China and Dr H. Felber of Switzerland were nominated as titular members. All members were asked about their eligibility status. A new member list will be circulated after the Geneva meeting. With the new Commission leadership, a special meeting in Tsukuba, Japan hosted by Prof. Okamoto was proposed for 1998. This meeting will serve to bring together the new titular members and officers to discuss and plan the future work of the Commission. With at least four laboratories participating as certifying laboratories, close communication and planning is vital for the programmes in progress. In addition, the newer members will be assuming more leadership roles and thus will need the advice and guidance of previous officers. A special budget request will be prepared for this meeting.

Review of the current rounds of the International Measurement Evaluation Programmes (IMEPs)

IMEP round 6—Trace Elements in Water

The active portion of this programme concluded in 1995. In addition to the previous publication, the results have been prepared for submission to 'Accreditation and Quality Assurance.'

IMEP round 7—Trace Elements in Human Serum

The samples have been received and distributed to the 'certifying' laboratories. The submission of samples to participants should occur early in 1998 with programme conclusion expected in 1998.

IMEP round 8—Carbon Isotope Ratios in CO₂

This programme will not begin until 1998 and is not expected to conclude until 2000. It is not listed with the current IUPAC Programme Information Files.

IMEP round 9—Trace Elements in Natural Water

Samples have been obtained and 'certifying' laboratories have been identified. Sample distribution would not begin until 1998, with the expected conclusion of the programme in 1999.

IMEP round 10—Trace Elements in Polyethylene

The necessary samples have been obtained and 'certifying' laboratories have been approached for measurements. Some measurements have begun. The programme is expected to conclude in 1999.

IMEP round 11—Trace Elements in Car Catalysts

This programme and a previously announced programme for trace elements in soils are both delayed and are not given in the current IUPAC Programme Information Files.

Future rounds under consideration

Action on these items is deferred until the special meeting to be held in Tsukuba in 1998.

The next meeting of the Commission will be held in Berlin in 1999. A special meeting of the major programme 'certifiers' will be held in Tsukuba, Japan in 1998.

Final report of the Working Party on Recycling of Polymers

The Working Party on Recycling of Polymers, consisting of 12 experts from 7 countries, was created by the Macromolecular Division (IV) in 1993. It held three meetings, produced 10 papers describing various aspects of the current state of polymer recycling, sponsored a Microsymposium on the same subject that took place in Prague in July 1997, and formulated a set of recommendations. The Working Party concluded its final work by correspondence.

The recommendations of the Working Party were adopted unanimously by the Macromolecular Division on 26 August 1997 at the IUPAC General Assembly in Geneva. The papers and the recommendations will be published together with the proceedings of the Prague Microsymposium on Polymer Recycling in

Macromolecular Symposia. On the recommendation of its chairman, the Working Party was then disbanded, having accomplished its assigned task.

Norbert M. Bikales
Chairman of the Working Party

Summary Minutes—Commission on Spectrochemical and other Optical Procedures for Analysis (V.4), of the General Assembly meeting, Geneva, Switzerland, 23–27 August 1997

Alignment for change

What is relevance? In terms of spectrochemical analysis, it means recommendations that get used and documents that meet real needs. To bring some of the many recommendations from V.4 into the light, several tactics were taken. First, our venerable chair Tuan Vo-Dinh, and John Bertie, the chair of I.5, wrote an article for *Applied Spectroscopy*, which presented the products of both commissions and described the objectives of the ongoing work. There has been strong positive response to the article, especially in the number of inquiries for reprints and preprints.

Secondly, all our documents were placed on the Internet at the IUPAC site on the RSC server (*Eds note:*

these have been moved to the new IUPAC web site at <http://www.iupac.org>). An introductory page was written containing the links to the various recommendations and provisional recommendations. As these are stored in PDF format, Acrobat Reader (available free) allows easy printing as originally published and complete text searching.

Thirdly, a number of relevant journal editors were approached to advertise the presence of the web site and the electronic forms of our documents, as well as to place a link to the site in their own web pages if they had them. All were extremely happy to do so. To produce useful documents that meet real needs, the pulse of technology-driven advances in optical methods for analysis continues to be taken by the members of V.4 and their contacts and colleagues. Yearly meetings and other venues are used to brainstorm about new projects deemed to meet some of these needs. Whether these be nomenclature documents to sort out confusion in newly developing fields or critical assessments to help researchers and analysts evaluate competing new technologies, the high energy of commission members is used to rapidly produce appropriate publications.

Next meeting: Commission members will convene at a mini-meeting during Europtode in Münster, Germany, 20 March 1998.

D.S. Moore, Secretary V.4