

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

Commission on Physical Organic Chemistry. III.2

Minutes of the twenty-fifth series of meetings held in Berlin
on 8-10 August, 1999

Meeting number: 88, August 8, 9.00-13.00
89, August 8, 14.00-17.00
90, August 8, 17.00-18.00 (with Div. VI and WP on Green Chemistry)
91, August 9, 9.00-13.00
92, August 9, 14.00-15.00 (joint meeting with Commission III.3)
93, August 9, 15.00-17.00
94, August 10, 9.00-13.00

Present:

Titular Members: Professor C. L. Perrin (Chair), Professor E. Baciocchi (Secretary), Professor J.-L. M. Abboud, Professor Z. Rappoport, Professor M.-F. Ruasse, Professor V. I. Minkin.

Associate Members: Professor S. S. Kim, Professor N. Nudelman, Professor R. Louw, Professor D. Lenoir, Professor P. Tundo (meetings 88-93), Dr. D. J. Raber, Dr. J. R. Zdysiewicz.

National Representatives: Professor R. S. Brown, Professor E. Uggerud, Professor T. M. Krygowski.

Observers: Professor T. Y. Luh, Professor E. M. Carreira, Professor E. P. Egorov (meetings 88-93), Professor P. Anastas (meetings 88-90), Professor T. Collins, Professor H. Zollinger (meeting 89, in part), Professor T. T. Tidwell (meeting 91, in part), Professor Y. Takeuchi (meeting 94), Professor J. Bradley (meeting 94).

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Minute 1/99. Opening remarks and approval of the agenda

The Chair welcomed the participants, in particular the observers. Each participant introduced him/herself. The Chair proposed some changes in the agenda which were approved.

Minutes 2/99. Minutes of the 24th series of meetings (Florianópolis)

The minutes were approved without changes.

Minutes 3/99. Report by the Chairperson and Restructuring of IUPAC

The Chairperson, Professor Perrin, reminded the Commission that the restructuring of IUPAC is under way. The briefing paper on this subject prepared by the Secretary General was summarized and distributed among the Members of the Commission. It was remarked that our Commission will dissolve in 2001 and that we are moving towards project-driven activities. There will be strong competition between projects since the budget of IUPAC is relatively small. In the wide-ranging discussion which took place, the risk was also pointed out that the new system will jeopardize the many voluntary contributions to IUPAC activities. Particularly, the precious contribution of the National Representatives may be seriously affected. It is hoped that in the Divisions there will be no limitation to the number of National Representatives. Doubts were also expressed about the possibility of an efficient recruitment of experts (Raber), which might also become difficult because the lack of an official status may be discouraging (Louw), particularly for young people (Lenoir). It was fully agreed that the future activity of our Commission will be devoted to the discussion of projects, which must be really good in order to meet the competition.

Minutes 4/99. Report by the Secretary

There was nothing to report.

Minutes 5/99. Project: Reactions, Pathways, and Processes in Green Chemistry

Professor Tundo reported on the activity of the Working Party on Synthetic Pathways and Processes in Green Chemistry and particularly illustrated a project on Green/Sustainable Chemistry for which he asks financial support on the basis of the new IUPAC system (see next item of the Minutes for details). There was some discussion concerning the use of the terms “green” or “sustainable”. The preference of the Commission was for “green”. It was also asked

whether there is any way to assess the degree of “greenness” of a chemical process, since a task of IUPAC should be that of giving guidelines in this respect. According to Professor Tundo, however, this is very difficult in view of the high complexity of the systems under observation. Prof. Tundo also briefly presented the draft of the White Book on Green Chemistry to be produced by the Working Party. This book will contain a Symposium-in-Print organized together with the Sub-Committee on Organic Synthesis chaired by Professor Black. Such a product should be published in *P&AC* as special issue. Professors Louw and Lenoir expressed some concern about the fact that the White Book might overlap with a book, entitled *Green Chemistry*, by Anastas and Warner published in 1998. The Commission was assured that this overlap will be less than 10%. Some discussion followed concerning the content of the White Book and the principles of green chemistry and several changes were suggested (and accepted) to improve some of the definitions.

Professor Louw introduced a topic concerning the teaching of environmental chemistry. This topic might be worthy of a specific project, of which Professor Louw presented a brief outline. In the following discussion it was remarked that such a project might have serious problems with both the Committee on Teaching Chemistry (CTC) and Division VI and that there are already several books on this subject. It was decided to postpone the discussion until the Commission considers the future projects concerning education (see Minutes 14/99).

Minutes 6/99. Joint Meeting with the Working Party on Green Chemistry and Division VI

This meeting was attended by Professor Miyamoto, Chairman of Division VI, Professor P. Anastas, Professor T. Collins, Professor W. Klein. Professor M. Herrken, Professor W. Anpo, Professor D. Black and, in part by the Secretary General, Dr. T. Becker. Professor Tundo illustrated the project on green/sustainable chemistry. He remarked that the project fits all (or at least 9) goals of IUPAC, addressing the following 6 points: 1) research and development; 2) awards and recognition on green/sustainable chemistry; 3) exchange of technical information related to green/sustainable chemistry; 4) guidance on activities and tools to support green/sustainable chemistry; 5) green/sustainable chemistry education; 6) improvement of the connection of IUPAC to society through green/sustainable chemistry activities. It was also noted that points 1-5 represent the 5 recommendations of the OECD (Organization for Economic Cooperation and Development) to the member countries. Professor Miyamoto assured that Division VI is ready to provide full support for this project. Different views were expressed about the establishment of priorities among the different lines of the project. Professor Perrin suggested that priority should be given to the aspects concerning research and development, education, and exchange of technical information. According to Professor Black the awards aspect also appears particularly important, especially for the OECD. Dr. Becker assured the Commission that the project will be approved, but he also wished to remind the Working Party that research projects should not be considered as they are not supported by IUPAC. The Working Party was fully aware of this point and accordingly its aim in this respect is only that of stimulating research and development.

Minutes 7/99. Project: Evaluation of Physical and Chemical Properties of Environmentally Important Organic Compounds

Professor Lenoir reported on the state of the project. It is still in an initial state, with no meeting of interested scientists yet arranged. Moreover, it is also feared that this project may be in competition with activities of Division VI. In this situation and considering that the project was required to be finished in the current year, the Commission expressed the opinion that the it should be abandoned.

Minutes 8/99. Project: Guidelines for Publication of Research Results from Empirical Force Field Calculations.

This project is finished and published in *Pure & Applied Chem.* **1998**, 70, 2047-2049. Dr. Raber will ask Journal editors to include these guidelines in the "Instructions for Authors".

Minutes 9/99. Project: Glossary of Terms in Supramolecular Chemistry

This project is still very incomplete, in fact, in a state not much different from that in 1998. Prof. O. Tee has turned over responsibility for the project to Prof. Tom Fyles. Much work remains to be done and it appears very unlikely that the project will be finished within one year. In order to make the product more authoritative it was suggested that the current version be sent for comments to the major scientists in the field of supramolecular chemistry.

Minutes 10/99. Project: Critical Compilation of Scales of Medium Effects

Part I of this project is finished and has been published in *Pure & Applied Chem.* **1999**, 71, 645-718.

Minutes 11/99. Project: Glossary of Terms Used in Theoretical Organic Chemistry

This project has been completed and was approved by Commission III.2 in 1998 for publication in *Pure & Applied Chem.* A provisional document has been distributed for review. The public comment period will end 31 October 1999.

Minutes 12/99. IUPAC on the World Wide Web

The use of the IUPAC Web site should be encouraged even though there is still some problem with access. The same encouragement goes to the use of e-mail for dispatching documents. The preferred format should be *RTF* even though it may require more space.

Minutes 13/99. Joint meeting with Commission III.3

The Chairman and the Secretary of Commission III.3, Professor J. Bolton and Professor R. S. Weiss, respectively, participated in this meeting. In connection with some general considerations on the restructuring of IUPAC, it was remarked that owing to its interdisciplinary character, the Photochemistry Commission should be directly connected to the Bureau or should constitute a Division of its own. Professors Perrin and Bolton briefly illustrated the projects going on in Commissions III.2 and III.3, respectively. In Commission III.3, projects are in progress or in planning which concern Photodynamic Therapy, Actinometry, Lithography, revision of the Glossary of Photochemistry, and Molecular and Supramolecular Photochemistry.

Minutes 14/99. Future Projects

Professor Nudelman presented a possible project on the **Environmental Degradation of Organic Compounds**. The aim of the project is the evaluation of the available information on the chemical and photochemical fate of organic pollutants in the environment (e.g., degradation of halocarbons in the atmosphere, degradation of pesticides, phenols, dyes, etc., in the aquatic environments and soils). It is expected to produce a document describing the most assessed pathways of degradation. The project was considered of great interest, but perhaps too broad. It was noted (Professors Abboud and Collins) that an entire book might be necessary for each pollutant. It was suggested that the project be limited, e.g., to reactions in water. Professor Nudelman accepted the suggestion, but noted that the project would deal with properties of classes of compounds, not of single products, since the degradation paths of single compounds

can be predicted through the use of free-energy relationships.

Professor Abboud reported on the possibility of preparing a second part of the **Critical Compilation of Scales of Solvent Parameters**. There are two problems. One is related to the existence of many empirical scales of solvent polarity and hydrogen bonding acidity and basicity. A compilation of this information might be of little utility and of short lifetime as it is very difficult to separate these contributions. The other is related to the important studies of medium effects by FT-IR carried out by Professor Laurence, which are reported only in a doctoral thesis. These studies cannot be ignored, but their use might not be appropriate for a critical compilation. Thus, Professor Abboud felt that further thinking is necessary before deciding to start with this project. Another project, however, might be considered: **A Critical Compilation of Hydrogen Bonding Acidity and Basicity Scales for Solutes**. According to Professor Abboud, several scales of this type are currently available and their critical revision can be carried out and could be very useful. The Commission endorsed this proposal even though it was remarked that a second part of the Critical Compilation of Solvent Parameters would also be a worthwhile project.

No progress has been made concerning a project on the **Bioorganic Glossary**. Professor Brown has contacted Professor Page but has not received any answer. Dr. Raber suggested that perhaps we should think of a Bioorganic-Bioinorganic Glossary. Likewise, no progress has been made in the study of a project concerning **Materials**. In this respect the Commission was informed from Professor Luh (National Taiwan University, observer) that he and Professor Beletskaya are organizing a Symposium in Print on Organic Materials.

For the preparation of a possible project on the **Acidity of Strong Acids** it was suggested that Dr. Cox and Dr. Raczynska be contacted.

An entire meeting (no. 94) was then devoted to the discussion of projects related to education, with the participation of Professors Bradley and Takeuchi of CTC. Most of the attention was dedicated to the project presented by Professor Nudelman to the IUPAC Secretariat according to the new guidelines. The project concerns an **International Organic Chemistry Curriculum**. Professor Nudelman explained that the main aim of the project is that of establishing updated Organic Chemistry curricula, which should facilitate exchanges of students and transferability of courses and curricula. A lively discussion ensued and several suggestions were made concerning the importance of the international aspect of the project, which should be more stressed, the distinction between students majoring and not majoring in chemistry, the importance of laboratory experience, and the exchange of teachers in addition to that of students. Professor Nudelman added that basically the project should establish what a student should know after a first year of organic chemistry (even if not majoring in chemistry). The Commission fully endorsed the project, but was informed by Professor Bradley that in general CTC is against too much standardization in chemistry teaching. Moreover, it was remarked that in the project there is too much emphasis on the input, whereas the outcome is not clear. It should also be considered that several universities may not meet the minimum indicated in the project and that complications might arise from the fact that in various countries there may be profound differences in the level of preparation of students when they enter university, which may require different curricula. Some attention should also be devoted to the similar efforts carried out in Europe in the direction of unification of curricula.

A discussion of the project proposal by Professor Louw concerning education in environmental chemistry (see minutes 5/99) had also been planned. Professor Louw, however, preferred to withdraw his proposal, thus there was no further discussion about it.

Minutes 15/99. Evaluation of projects

In the light of the project-driven future activity of IUPAC, an evaluation of the projects carried out in the past by the Commission was considered appropriate and potentially very useful. It was decided that a first approach to this goal might be a self evaluation, i.e., the members of the Commission would judge the projects produced by the Commission itself in terms of familiarity and use. This approach was carried out and the documents judged most favorably were: the Glossary of Terms Used in Physical Organic Chemistry, the Critical Compilation of Scales of Medium Effects, the Compilation of Substituent Constants, and the Symposium-in-Print "Physical Organic Chemistry in the 21st Century". Of course, other, more objective, systems to evaluate the projects should be devised. It was suggested that for the documents in the IUPAC Web site, the number of contacts might provide a quite reliable criterion to judge the usefulness and the impact of the document.

It was also remarked that some documents (e.g., the Jencks notation) have had a quite limited impact. It was suggested that the documents produced by the Commission should be sent to potential authors of books on organic and physical organic chemistry. It would greatly contribute to their diffusion if the documents were mentioned in these books.

Minutes 16/99. Membership.

It was proposed and agreed that membership be extended to 2001 for all Members of the Commission.

Minutes 17/99. Future Meetings

Professor Ahlberg has sent a report concerning the organization of the 15th ICPOC in Göteborg, Sweden. The Conference will take place on July 8-13, 2000. The financial situation is good. It was unanimously approved that the 16th ICPOC will take place in 2002 in San Diego, USA. Applications are solicited for the 2004 and 2006 Conferences, particularly from Spain, eastern European countries, and China. It was agreed that an open meeting of Commission III.2, or of whatever body succeeds it to organize IUPAC activities involving physical organic chemistry, will be held at each ICPOC conference.

Minutes 18/99. Other business

There was no other business arising.

Minutes 19/99. Closing remarks

The Chair thanked all participants in the meetings for their contributions. A strong complaint was also expressed about the inefficiency of the local organization.