**Minutes of the Meeting of the Commission on Chemical Kinetics - I.4**
**Division of Physical Chemistry**
**40th General Assembly IUPAC, Berlin, Germany**
8-9 August 1999

Present: *Titular Members: Dr. M. Rossi (Chairman), Dr. J. T. Herron (Secretary), Prof. D. L. Baulch, Associate Members: Dr. T. Bérczes; National Representatives: Prof. E. Breet, Dr. E. B. Ljungström; Observers: Prof. A. Gellman*

## A. Report of the Chairman

The Minutes of the last General Assembly meeting held in Geneva, Switzerland, 24-25 August 1997 were approved.

The Chairman opened the meeting by outlining the new structure and mission of IUPAC that would be put in place following the next general Assembly. The key elements, such as the move to a project based structure and the reduction in costs of the General Assembly were discussed in some detail; the general consensus of the members being that the new structure could lead to a more vigorous and accountable organization. However, questions as to how, for example, the members of the new Division Committee would be appointed remain unanswered at this time

The Chairman emphasized that although the new structure would not be in force until after the next General Assembly, it was critical to make changes in operational procedures now. In particular, it was noted that every effort should be made to complete projects before the end of the next biennium. Projects extending beyond 2001 would need to be re-submitted to the secretariat.

## B. Status of On-Going Projects

140/6/93. Evaluated Chemical Kinetic Data for Combustion Chemistry

Prof. Baulch reported on the status of this project, the starting points of which were the evaluations carried out and published previously by a non-IUPAC panel (J. Phys. Chem. Ref. Data, **21**, 1125 (1992); **23**, 847 (1994)). As reported at the last meeting, a working party was organized and specific evaluation tasks assigned. Approximately 90% of the assigned tasks have been completed, and the balance is underway; a manuscript is expected to be completed in early 2000. It was also pointed out that the confluence of experiment and theory made it highly desirable to add someone with a strong background in theory to this group.

Funding to support the task group members has now been exhausted, and new funding sources are needed to carry on this ongoing project. In particular, secretarial and clerical support services are needed to unify the contributions of the different contributors. In addition, it will be necessary to find a successor to Prof. Baulch as a task leader for this project.

140/7/93. Aqueous Solution Kinetics Data for Atmospheric Chemistry

In the absence of Dr. Huie, there was no detailed report on the progress of this project, which is a joint activity with the Commission on Atmospheric Chemistry (VI.2). Dr. Herron

reported that it had been hoped that the project could be carried out through the use of the Internet rather that though periodic participant meetings. However, difficulties in putting that approach into practice have delayed implementation.

140/8/94. Task Force on the Thermodynamic and Chemical Data Base for Hazardous Waste Processing

Dr. Herron reported that after much delay, the project would be completed this year. It is planned to issue a report, but not to proceed to publication through PAC. A brief summary will be made for Chemistry Today.

140/9/97. Evaluation of Thermodynamic Properties of Selected Free Radicals

Dr. Bérczes reported that the data for inorganic radicals was well in hand. For organic radicals, a recent publication has addressed many of the issues that engendered the study. The major remaining area of uncertainty, the properties of larger organic radicals (3 or more carbon atoms) and the unsaturated radicals, is still an active experimental and theoretical problem area, and is not yet mature enough to be the subject of a data evaluation.

There is a project underway at NIST, in support of the NASA Data Panel, on the thermodynamic properties of free radicals of importance in atmospheric chemistry which is addressing some of these issues. It might be possible for IUPAC to provide some support for this work (not through direct funding), and extend it to larger radicals. A project leader would need to be appointed and supported in some fashion to do so. Dr. Herron will discuss this project with Dr. Huie at NIST and report back to the Chairman.

Prof. Bérczes has agreed to undertaking the preparation of a brief document on data needs in the area of free radical thermochemistry from the point of view of the chemical kinetics user community. This summary of pertinent questions in regards to the thermodynamic properties of small free radicals may also be of great value in initiating a potential new project with the theoretical chemistry group dealing with computational aspects and prediction of thermodynamic properties of small free radicals and other critical reaction intermediates.

140/100/97. Kinetics Data for Chemical Processes under Extreme Conditions

Prof. Breet reported the results of his feasibility project on Kinetics Data for Chemical Processes under Extreme Conditions. He identified seven areas of chemistry with strong conceptual and data needs. Of these, two were highlighted for immediate attention: sonochemistry and supercritical fluid chemistry.

The applications of these areas were outlined. It was the general consensus that there was now a clear need to proceed by organizing a workshop on data and application needs. The first topic area to be addressed would be supercritical fluids. Prof. Breet agreed to contact the experts in various aspects of the subject and to investigate the mechanism for organizing a workshop before the next assembly.

141/3/89. Kinetic, Photochemical, and Heterogeneous Data Evaluation for Atmospheric Chemistry

Dr. Rossi reported on progress on the continuing series of data evaluations for atmospheric chemistry. The most recent supplement (number V) was completed in early 1995, but published only in early 1997 (J. Phys. Chem. Ref. Data, **26**, 509-1011, 1997) due to problems in the journal production process. Supplement VI and VII have been published (VI: J. Phys. Chem. Ref. Data **26**, 1329-1499, 1997, VII: J. Phys. Chem. Ref. Data **28**, 191-393, 1999 and Supplement VIII has been submitted to the Journal of Physical and Chemical Reference Data. Supplement IX dealing exclusively with heterogeneous reactions is expected to be submitted in electronic form to a WEB site (http://www.iupac-kinetic.ch.cam.ac.uk/) in the near future with Supplement X (heterogeneous reactions only) to follow soon thereafter. The most recent publication is the sixth major data evaluation published in this series, which is extensively used in mathematical models of the stratosphere and troposphere. Summaries of the evaluations are available at a web site: http://www.iupac.org/divisions/I/cp1.html.

**C. Continuing and New Projects**

It was agreed that the three current data projects, Evaluated Chemical Kinetic Data for Combustion Chemistry, Aqueous Solution Kinetics Data for Atmospheric Chemistry, and Kinetic, Photochemical, and Heterogeneous Data Evaluation for Atmospheric Chemistry, because of their great impact on modeling the production and control of environmental pollutants, would be continued through the next biennium.

On the basis of the presentation of Prof. Breet, it was decided to continue the project Kinetics Data for Chemical Processes under Extreme Conditions, with a focus on supercritical fluid kinetics. As noted above, Prof. Breet has agreed to explore the feasibility of organizing a workshop to focus on this topic and to provide guidance to the commission as to organizing a formal data project.

**D. Elections**

Dr. M. Rossi was re-elected Chairman and Dr. J. Herron, Secretary. Profs. D. Baulch and J. Troe and Dr. R. Huie agreed to serve as Titular Members, and Profs. Tibor Bérczes and John Plane have agreed to serve as Associate Members through 2001. Prof. E. Breet was elected as a new Titular Member.

The roster of the Chemical Kinetics Commission for the biennium 2000-2001 is as follows: Titular Members: Prof. D. Baulch, Prof. E. Breet, Dr. J. Herron, Dr. R. Huie, Dr. M. J. Rossi, Prof. J. Troe; Associate Members: Prof. V. Azatyan, Prof. T. Bérczes, Prof. J. Plane, Prof. P. Van Tiggelen.

The list of National Representatives presented by the Chairman was approved.

**E. Next Meeting**

The next meeting of the Commission will be held in Brisbane, Australia, on 1-6 July 2001.

**F. Meetings with Other IUPAC Groups**

1. Meeting with Commission on Fundamental Environmental Chemistry (VI.1).

Although the focus of Commission VI.1 is on bulk properties relating to major environmental transformations, there are some areas of mutual interest which have potential for collaboration. These include heterogeneous kinetics, the chemistry of hydrothermal vents (of particular interest in terms of the proposed new activity in Commission I.4 in extreme conditions), redox reactions, and autocatalysis. A suggested joint activity would involve a workshop on the chemistry of hydrothermal vents.

2. Meeting with Commission on Atmospheric Chemistry (VI.2).

The current status of the joint project Aqueous Solution Kinetics Data for Atmospheric Chemistry was discussed. It was agreed that his project was of great importance and should be continued within Commission I.4, and that as the work progressed, reports be sent to Commission VI.2 for comment and input. It was pointed out that some aspects of that project were already in hand, such as data on Henry's law constants.

Other areas of mutual interest were discussed, such as chemistry on soot particles, sulfur dioxide chemistry, and nitrate radical chemistry.

3. Meeting with Commission on Photochemistry (III.3).

There are many areas of interest to Commission III.3 which involve fundamental kinetics data, such as UV disinfection, lithography, and single molecule photochemistry. Also, Commission III.3 serves as the primary source of information on correct terminology and symbols within IUPAC. They volunteered to act as readers for data works involving photochemical quantities.

4. The Chairman also met with the Subcommittee on Theoretical Chemistry of the Commission on Molecular Structure and Spectroscopy (I.5).

**G. Concluding Remarks**

The members of the Chemical Kinetics Commission are looking towards the future with confidence and optimism knowing that they will successfully meet a dual challenge awaiting them:

- The projected and slimmed-down organization of IUPAC centered on project driven management which will offer significant opportunities to further the cause of chemical kinetics, both within the Physical Chemistry Division as well as within the general scientific community, and
- The role of the WEB in the publication and dissemination of all types of scientific information from general survey-type to detailed research accounts and its possible specter of displacing to some extent the traditional means of scientific publishing.