

## Meeting of the Commission on Biophysical Chemistry (I.7)

Berlin, Germany. August 8-9, 1999

Members of the Commission who attended the meeting are:

Helmut Hauser - Chairman  
Robert Goldberg - Secretary  
Hans-Jürgen Hinz  
Frederick Schwarz  
Daniel Thévenot  
Kurt Wüthrich

Two observers from the National Research Council (NRC) were also present. They were James Cowan and Richard Goldstein.

Note: not all members of the Commission were present for the entire meeting.

### 1. Discussion of Agenda.

Topics of business to be discussed included: (1) project review; (2) feasibility studies; (3) future directions; and (4) membership. The schedule of presentations of specific items and the matter of joint meetings with other Commissions were also discussed.

### 2. Overview of Developments in IUPAC and within I.7.

Helmut Hauser discussed the project oriented reorganization that will take place within IUPAC. This reorganization will eliminate the Commissions and substitute a system that is project oriented. However, it will still be possible for the Division Committees to institute structures and task groups at its discretion. The Division Committees will make the final decisions on which projects are initiated as well as the amount of funds that the projects will receive. Robert Goldberg reported on what he learned from Ted Becker's recent address to the NRC on the changes taking place within IUPAC. The general aim is to identify and to support good projects. Helmut Hauser reported that the Commissions will continue until December 31, 2001 and thus will still be in existence for the next General Assembly to be held in Brisbane, Australia in 2001. The budget of I.7 will be approximately 7000 US\$ for the next biennium.

There was also a general discussion of funding of projects. The question of just what amount of funds could be obtained from IUPAC was raised. It was also pointed out that funds could sometimes be obtained from other organizations (i.e. CODATA, NSF).

Kurt Wüthrich pointed out that I.7 was different from several other Commissions in that we were not working together on a single project. Instead I.7 oversees several individual projects. Kurt also emphasized the importance of having I.7 properly represented at the Division level.

Kurt Wüthrich will become the Chairman of I.7 on January 1, 2000 and will serve in this position until December 31, 2001. After that date I.7 will cease to exist.

Kurt Wüthrich also mentioned that "Recommendations for the presentation of NMR structures of protein and nucleic acids" that was written by the IUPAC-IUBMB-IUPAB Inter-Union Task Group was published in several journals:

Pure and Applied Chemistry, the Journal of Biomolecular NMR, and in the European Journal of Biochemistry, and Biochemistry.

### **3. Joint meeting with Commission V.5 (Electroanalytical Chemistry Commission)**

Daniel Thévenot reported on his project on Electrochemical Biosensors. He has incorporated several revisions to this document that dealt with conditions for assessing the performance of biosensors and the reproducibility of results. The issue of single-use devices was raised, i.e. how they should be calibrated and also what they should be called. The general recommendation of those present was that these devices should be called "single-use" to distinguish them from other devices that should be designated "multiple-use." This issue of terminology is an issue that Daniel Thévenot has to resolve with his co-authors. There also has to be some coordination with Commission V.4 which has produced a related document. It was agreed that this project would be complete once these few remaining matters could be resolved.

Later in the meeting and following discussions with members of V.4 and with George Wilson, Daniel Thévenot reported that there will be some uniformity in the classification of optical and electrochemical biosensors. Also, George Wilson recommended the use of the terms "single-use" and "multiple-use." Daniel Thévenot also reported that the issues related to selectivity, stability, drift rate, and lifetime have been resolved. Thus the publication on biosensors is essentially ready for approval by IUPAC and then for publication in Pure and Applied Chemistry.

### **4. Joint Meeting with Commission I.3 (Electrochemistry)**

George Wilson reported for Fred Hawkrige on the status of the project "Redox Potential Measurements of Proteins." At present Fred is very much preoccupied with his work at NSF as well as being the chairman of the Chemistry Department at Virginia Commonwealth University. Therefore, there was not much progress to report on. Nevertheless George Wilson stated that their document was in a semi-final form and that he would make a very serious effort to complete the project by the end of 1999. He also reported on the serious scientific issues associated with this project, i.e. the issue of whether or not the system is at equilibrium and the fact that the measured emfs depend on ionic strength, buffer, and pH. Additionally there is a very fundamental issue of what model and data to use for the activity coefficients of macromolecules. George Wilson also stated that some of the more difficult aspects of the project could be dealt with in future projects. The current project will deal with the more practical issues involved in these measurements, but will not carry IUPAC recommendations.

George Wilson is also the President-elect of the Physical Chemistry Division and gave some perspective regarding future activities. He stated that Biophysical Chemistry would very likely become a major IUPAC activity. He intends to bring new people with the appropriate background into the Physical Chemistry Division Committee. He also discussed the matter of funding for future IUPAC projects as well as the crucial issue of attracting the best people to undertake these projects. In the absence of large grants for IUPAC projects, it appears that "good citizenship" on the part of scientists, the desire to bring some needed unification to a field of research, some limited financial support, and some prestige will be the likely motivating factors for those undertaking IUPAC projects. George Wilson emphasized that the current situation remains very fluid and that many matters still need to be resolved. These matters include the membership of the Division committees after 2001, how often they will meet, and how often and where the various task groups will meet.

## **5. Report on Status of Project on Differential Scanning Calorimetry (DSC)**

Hans-Jürgen Hinz and Fred Schwarz reported on the status of their project "Recommendations for the Measurement and the Analysis of Results Obtained on Biological Substances with Differential Scanning Calorimetry." Hinz and Schwarz reported that their document is very close to its final form. A major addition to the previous version is the inclusion of experimental results for lysozyme unfolding which were obtained from several laboratories. The final document contains a discussion of the basis of DSC as applied to biochemical denaturations, how one should use these instruments, and how results should be analyzed and presented in the literature. Hinz and Schwarz have received comments on the document from several researchers and plan to distribute copies of it to additional persons at the U.S. Calorimetry Conference which is scheduled to begin August 15, 1999. They will then make necessary revisions to the document and submit it to the Chairmen of I.2 and I.7 for approval of its publication in Pure and Applied Chemistry. This document was also discussed in the joint meeting with Commission I.2.

Hinz and Schwarz also discussed a proposed project on isothermal titration calorimetry (ITC). ITC is currently in wide use and may very well be the single most widely used method for the determination of binding constants and enthalpies of reaction. However, since there are a significant number of people using these instruments who have little background in calorimetry and thermodynamics, there is a real need for an authoritative discussion of ITC. The proposed IUPAC project would be similar in structure to the document on DSC and give background on the measurements, analysis of results, calibrations and test reactions, and recommendations regarding procedures and reporting of results. Hinz and Schwarz agreed to draft a project initiation document. Robert Goldberg would assist in this matter as needed.

## **6. Terminology in the Field of Lipid Vesicles (Liposomes).**

Helmut Hauser reported that this project would have been completed except for the untimely death of Dimitri Papohadjopoulos, a key member of the working party. In spite of this setback, this project is almost complete. Helmut Hauser stated that it would be completed and submitted to Pure and Applied Chemistry by the end of 1999.

## **7. Nomenclature for Lipid Mesophases.**

While Martin Caffrey was not present for this meeting, he did report to Helmut Hauser on the status of this project. Thus, the report on this project was given by Helmut Hauser. Essentially, very little has been accomplished. Martin Caffrey attributed the lack of progress to the absence of the prerequisite funds. The IUPAC funds that this project received were used to support two meetings of the working party. Martin Caffrey will continue this project only if adequate funds are received. Since the funds needed significantly exceed the amount that IUPAC grants for projects, the continuation of this project is dependent on funds from other sources, e.g. NSF. The consensus of those present was that Martin Caffrey should be encouraged to seek funding from NSF and to complete the project by 2001.

## **8. Meeting with Tom Cvitaš, President of the Physical Chemistry Division**

Tom Cvitaš encouraged those seeking funds for future IUPAC projects to apply for them as soon as possible. These funds can be used to support existing

projects. There was some general concern as to how the Physical Chemistry Division will deal with Biophysical Chemistry. Tom Cvitaš gave some general encouragement for the future of Biophysical Chemistry within the Physical Chemistry Division and within IUPAC. He urged the submission of suitable and important projects in this discipline.

#### **9. Computations in Biophysical Chemistry.**

Terry Stouch was not present at the meeting and no report has been received from him. Nevertheless, there was some general discussion of the potential importance of this project. However, Kurt Wüthrich expressed some reservations about the membership of the working group as well as the lack of a report from Terry Stouch on the project. Helmut Hauser will contact Terry Stouch about the status of the project.

#### **10. Membership of I.7**

The membership of I.7 will undergo a dramatic change on December 31, 1999. Kurt Wüthrich will become the Chairman. Helmut Hauser will no longer be on the Commission and Robert Goldberg will have completed 12 years and will also retire from IUPAC. The other TMs are Fred Schwarz and Hans-Jürgen Hinz; their appointments also expire. Kurt Wüthrich expressed his concern about the lack of continuity in I.7 and suggested the possibility of seeking to keep Robert Goldberg for two more years as Secretary and to maintain some continuity and perspective in I.7. Helmut Hauser also proposed the removal of those AMs who have made no contribution to I.7 or to IUPAC.

#### **11. Joint meeting with Commission 1.2 (Thermodynamics)**

Several topics related to biophysical chemistry and to thermodynamics were discussed. These included buffers for biochemistry and biology, DSC, Standards for isothermal microcalorimetry, and ITC.

Kip Murphy was to have presented a feasibility study on a project on buffers for biochemistry and biology. He, however, was not present and no feasibility study was presented. There was some general discussion of this subject and there was a general consensus that this could be a very useful and important project. Robert Goldberg stated that the proper completion of this project would require a substantial effort and should not be undertaken without such a commitment. Daniel Thévenot also raised the issue of how buffers interact with biochemical substances - both substrates and buffers. Ron Weir stated that he would contact Kip Murphy about the status of this project.

Fred Schwarz again reported (see item 5 above) on the status on the project "Recommendations for the Measurement and the Analysis of Results Obtained on Biological Substances with Differential Scanning Calorimetry." Several members of I.2 requested that Fred Schwarz send them copies of the pertinent document.

Ingemar Wadsö is the coordinator of a group that has prepared a draft copy of "Standards for Isothermal Microcalorimetry." This document deals with some aspects of ITC a subject which is of direct relevance to the project that Fred Schwarz and Hans Hinz plan to submit to IUPAC. Ingemar Wadsö plans to hold a workshop on standards for biological calorimetry at the International Conference on Chemical Thermodynamics that will be held in Halifax, Nova Scotia in the year 2000.

## **12. Possible Future Projects**

In addition to the project on isothermal calorimetry (coordinators: Hinz and Schwarz), other possible future projects were discussed. Specifically, there was some discussion of the future of the project dealing with guidelines for publication of results obtained using various methods of molecular mechanics and force fields (coordinator: Terry Stouch). It was felt that a more appropriate title was needed for this project. While there was a very brief discussion on possible projects dealing with irreversible thermodynamics and with kinetics, no specifics were proposed. Finally, there was some discussion of databases. Kurt Wütrich expressed his concern about the handling of very large databases such as the Brookhaven database. His concern was that such projects should be well maintained and properly run; he was not convinced that proper funding for such a large project was available to assure its proper continuity. Suitable coordinators must be found if projects in irreversible thermodynamics, kinetics, and databases are to become IUPAC projects.

## **13. Joint Meeting with I.6 (Colloid, Surface Chemistry, and Catalysis)**

General summaries of the projects in I.6 and in I.7 were presented by Luuk Koopal and by Helmut Hauser, the respective chairmen of these Commissions. The project that evoked the most general interest was the project on computational chemistry. There was a general consensus for the need for a set of guidelines for the presentation of the results from computational chemistry. At present even the experts in theoretical chemistry often have difficulty understanding and reproducing the computational results of others.