



**PHYSICAL AND BIOPHYSICAL CHEMISTRY DIVISION REPORT**

**2000-2001 BIENNIUM**

May 2001

Summary

The Physical and Biophysical Chemistry Division (PBPCD) has been actively engaged in preparing for the transition to the project-based organization that will take effect at the beginning of the next biennium.

- *Change of Division Name* - By action of the Bureau in September 2000 the name of the Division was changed to *Physical and Biophysical Chemistry*. This change was prompted by the desire to emphasize that biology is after all chemistry, and to recognize the interactions of the Division with other Unions in the area of physical characterization of biologically-important molecules. Especially important are spectroscopic techniques that will play an important role in the rapidly developing area of proteomics, for example. The efforts of the Division will be coordinated with those of Division III, where other aspects of biomolecular chemistry and biotechnology will be managed.
- *Structure of the Division Committee* - Because the Division has historically been very large (7 commissions and 6 sub-committees), there is considerable concern that the disappearance of the commissions will have a negative effect on continuity. The commission chairmen will no longer assume the administrative role so essential to keeping projects moving. Since the Division Committee (DC) must now assume these responsibilities, we have attempted to strike a balance in membership between persons with IUPAC experience and those who can bring "fresh" ideas for the future. The DC elections for the 2002-2003 Biennium were recently conducted by the Secretariat. Elections were held in advance of GA so that the newly-elected members could attend the DC meetings in Brisbane and thus be prepared to immediately assume responsibilities when their terms begin in 2002. As a result of these elections, the DC for the next biennium will have 5 persons who have recently served as commission chairmen, 5 persons who have mostly no experience in IUPAC, and two officers with extensive IUPAC experience. The newly-elected members have a high profile in the chemical sciences community, and it is expected that they will aid in expanding our constituency in devising more effective ways to disseminate the activities of IUPAC. The DC constituted for the next biennium will have 12 TMs including four officers and the chairman of the renewed Commission I.1 (decision pending) No decisions have, as yet, been made concerning AMs and NRs.
- *Quantities, Units and Symbols in Physical Chemistry* - By analogy to chemical nomenclature, it is extremely important to have a compendium of symbols, units and quantities that are self-consistent and widely accepted. Commission I.1 has, in the past, had responsibility for this activity. Members of this commission have served on the IDCNS in monitoring recommendations for projects across the Union. Continuation of this Commission has been requested so that it can provide both continuity and authority within and also outside IUPAC. This hard-working group is now in the final stages of production of the 3<sup>d</sup> Edition of the Green Book.
- *Project Management* - At present there are 35 active projects within the Division. Four have so far been completed. This is clearly too large a number to maintain in the future, and therefore we are making a strong effort to complete by the end of the present biennium all projects that merit completion. No projects will be

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continued beyond December 2001, and no new projects will be initiated unless they have passed through the new review system. So far four projects will be carried forward. Two are new projects and two are continuations of on-going projects. We have been very cautious about initiation of new projects until we have had the opportunity of discussing in more detail as a group the strategies for the next biennium. The project management structure must be flexible, and we are still discussing how this might be implemented.

- *Continuity* – As noted above, the loss of persons with lots of experience in IUPAC projects is a matter of great concern. To be sure they can be included as part of Task Groups and therefore continue to provide important advice. Up to a point, input can be obtained by E-mail and therefore interactions can be rapidly and efficiently implemented. Still, many want to feel that they are a more integral part of the continuing activities of IUPAC. The IUPAC Fellow program will help, but the Division is planning to set up a data base at the Secretariat designed to make available the names and interests of members of the chemical sciences community so that if the institutional memory fails, we will still be able to identify and involve former members of the Division not presently on the Division Committee. It is expected that this database could also include people who are interested in IUPAC, but have had no opportunity to participate in its activities.
- *Project Activity During the Current Biennium* – The various projects carried out during the present biennium are listed in Appendix 1. These projects generally fall into three categories: 1. Preparation of Critically-Evaluated Databases; 2. Specification of methods, components and parameters for describing and reporting on experimental results using a variety of techniques; and 3. Workshops. In two areas in particular, thermodynamics and atmospheric chemistry, there is a need for compendia of data that can be considered reliable. Such information is particularly valuable to industry and to various government agencies charged with the responsibility for environmental monitoring and assessment. Such tasks can only be carried out by well-organized and experienced scientists. In the second category can be found conventions for reporting experimental results. Journal editors are very reluctant to require authors to conform to particular conventions, however, they have sometimes proven willing to reprint recommendations initially published in PAC. Alternatively, they have been more willing to provide links between the Web pages of the journal and IUPAC. In the Appendix will be found several examples of manuscripts that have been reprinted several times. Workshops have been used as a basis for bringing together groups to focus on specialized issues. The usual requirement is that a report is prepared so that others can benefit from the exchanges that have taken place.
- *Dissemination* – The need to more aggressively promote IUPAC and its activities is obvious. If we can provide rapid access to useful information, the role of IUPAC in making such information available will be more obvious. Consequently, a Web version of the Green Book is planned. Also, some, but not all of the groups involved in critical evaluation of databases have concluded that such information should be put directly on the Web so that scientists will have an up-to-date and readily accessible body of information. It will not be necessary to seek out the original papers and the associated addenda. However, there remain a variety of problems associated with information in electronic form, and these will have to be worked out by IUPAC as a series of general policies.

### **Biennium Report**

#### **Current Activities**

During the present biennium, the Division has continued to emphasize two of the task areas to which it has assigned the highest priority: definition of quantities, units and symbols (Green Book), and critical evaluation of databases. This emphasis is consistent with the strategic thrust of IUPAC in the direction of providing tools for scientists to use and in enhancing communication by making our language more specific. In

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preparing the 3<sup>rd</sup> Edition of the Green Book considerable effort has been expended to put the text in a format that is Web compatible, the main problem being the need to generate symbols that are beyond the capability of most word processing programs. The final proofreading of the text is underway, and this new version should be ready for printing in the next several months. A version of this new text is envisioned for the IUPAC Web site. We believe that this will be a very effective way of encouraging students in particular to use the correct quantities and symbols. Recently the European Community has begun to insist that SI units be used in patent applications, and it is likely that as the global markets continue to expand, there will be increasing pressure for uniformity. In the preparation of the new edition of the Green Book, significant effort was devoted to the balance between development of a consistent system of notations, and one which scientists in particular fields will actually use. As noted, getting this material on the Web is considered a key step in the dissemination of this important information.

Some symbols and quantities are so specialized that they do not appear in the Green Book and thus recommendations are published in PAC. This is not sufficient. Thus Commission I.5 (Spectroscopy) has been successful in getting recommendations concerning NMR and Fourier Transform spectroscopies either republished in other journals or linked to the IUPAC Web site. Recommendations for biosensor definition and classification have been similarly republished.

Commission I.2 (Thermodynamics) has been active in the critical evaluation and publication of data relating to the properties of organic solvents, including vapor-liquid critical properties, thermal conductivity, and viscosity. In addition, a series of monographs on conductivity and transference numbers of ionic species in organic solvents have recently been published. A monograph on Chemical Thermodynamics was published as part of the series, Chemistry for the 21<sup>st</sup> Century. Contributions from a wide range of authors served to demonstrate the relevance of this field to modern science. The Chemical Thermodynamics group has chosen to disseminate their databases in the form of print publications. Commission I.4 (Kinetics) is involved in the evaluation of gas kinetic data that is of relevance to the study of combustion and to reactions in the atmosphere. They have chosen to deposit their data on a database at the University of Cambridge, and this is directly linked to the IUPAC Web site. They have been working closely with a small National Aeronautics and Space Administration (U.S.) (NASA) group to coordinate the atmospheric data evaluation effort.

The Division has also been active in issues relating to the environment. For example, the Second International Workshop on Thermochemical, Thermodynamic and Transport Properties of Halogenated Alkanes and their Mixtures took place in Fontainebleau, France, April 9-11, 2001. There were 120 participants with 11 invited lectures, 27 oral presentations and 60 posters. About 30 selected papers from the Workshop will be published in a Special Issue of Fluid Phase Equilibria in 2002 with J.H. Dymond and D. Richon as editors. This focus is clearly relevant to the issue of halogen-containing compounds in the atmosphere. Commission I.4 has provided critically-evaluated data for such species. A Workshop sponsored jointly by IUPAC and ICSU, "Electrochemistry and Interfacial Chemistry for Environmental Clean-Up and Green Chemical Processes" was held in Coimbra, Portugal April 6-7, 2001. There were 77 participants from 18 countries, and an introductory half-day tutorial session was given prior to the start of the Workshop, thus providing an educational component to this important area. This activity was coordinated by Commissions I.3 (Electrochemistry) and I.6 (Colloid and Surface Chemistry). A technical report for PAC is planned and publication of the proceedings is also being considered. The Sixth International Conference on Inorganic Membranes took place in Montpellier, France June 26-30, 2000. A technical report is forthcoming from that conference as part of a joint effort with Division II (Inorganic). Commission I.6 used the occasion of the International Conference on Electrokinetic Phenomena to obtain input from the scientific community that will form the basis for the revision of a document in this area currently under revision.

The Division is actively engaged in horizontal interactions within the Union. We are participating in initiatives in the areas of the environment and in advanced materials.

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### Future Plans

As noted above, an effort will be made to maintain fewer projects within the Division, but with higher levels of support for some projects. As a result of interactions between the Subcommittee on Theoretical Chemistry and Commission I.4, a new project has evolved, "Selected Free Radicals and Critical Intermediates: Thermodynamic Properties from Theory and Experiment". This is a Task Group consisting of six experimentalists and seven theoreticians from seven different countries. Their first task was to identify organic free radicals that play an important role in atmospheric chemistry and/or combustion. These two groups of scientists, who would normally not be talking to each other, are critically evaluating experimental thermodynamic data and establishing by high level *ab initio* calculations whether the experimentally determined parameters are logical and consistent. There is even a research component to the project that makes it interesting and challenging to the participants.

A second project involves the continuation of an on-going project (141/3/89) involving the evaluation of gas phase reactions in the atmosphere. The goal will be to have a database that is easily maintained, is user friendly, and can be easily updated to include new or revised data.

In addition, we will have several small projects supported from the Division budget. However, we will be devoting considerable effort at the Division Committee level to the development of new ways to identify appropriate projects and to more effectively engage the chemical sciences community in their development.

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Physical and Biophysical Chemistry Division