Introduction to the Special Issue "Thermodynamics of Hydration"

The offer to organize and edit a Special Issue of *Biophysical Chemistry* came to me early in 1993 from the Publishing Editor of Elsevier Dr. Kostas I. Marinakis through mediation of Dr. Peter L. Privalov, who had initiated the idea. I want to thank both for this exciting opportunity.

In the following discussions we agreed that the field of hydration thermodynamics is of central importance to both biophysics and physical chemistry, and it is also full of controversies and conflicting points of view. Any progress in their resolution may have serious impact not only on basic science but also on its applications in bio- and chemical technologies. Therefore we decided to invite specialists representing contrasting opinions and diverse branches of the field to participate in the Special Issue.

Further dwelling on the organization of the Special Issue led me to the idea that it could be interesting to not only collect papers representing diverse opinions and approaches but to allow the participants to comment on each other's contributions and respond to the comments. Such comments and responses, published along with the papers, would allow to highlight problems that are usually swept under the rug, and to attempt a development of a common language by practitioners of diverse techniques and adherents of contrasting points of view. This could also allow to effectively have a journal conference without holding an actual physical meeting, and to stimulate involvement of the readers in the budding of new ideas and in their development. The idea of such Discussion was supported by prospective participants and actually made this Special Issue possible despite a heavy load of other writing commitments carried by its many participants. And, to tell the truth, we expected to have good scientific fun.

To assure high scientific quality of the Special Issue all of the contributions were subjected to the normal pear review. Most of the reviews were solicited from scientists who did not participate in the Issue. A few late papers were subjected only to the editorial review within the field of expertise of this editor (the papers by R.M. Levy, E. Freire, second paper by V.V. Nauchitel and R.L. Somorjai, and B.K. Lee's paper on the role of hydrogen bonds in hydrophobicity). Negative reviews based on partisan prejudices were rejected. Doing otherwise would prevent an exposure of conflicting opinions.

The result is quite satisfying in our opinion. There are 23 papers in this Issue from 18 individual scientists or scientific groups, 16 of which are followed by discussions ranging in length from 1 to over 10 typewritten pages. Controversial papers and papers from groups expressing contrasting opinions apparently produced the longest discussions. A variety of subjects has been covered. The paper by Barone et al. reports new experimental results on hydration of N-acetyl amino acid amides. The paper by A. Ben-Naim is devoted to a 'correct' way of deriving at experimental values of the free energies of hydration. The paper by Chalikian et al. reviews studies of partial compressibilities of biological compounds. R. Cachau describes a modern approach to the

molecular dynamics program for parallel computers using look-up tables instead of analytical functions representing interaction potentials. E. Freire uses results of experimental measurements of hydration to describe the structure of a molten globule intermediate in the folding of barnase. J. Gao applies the combination of empirical quantum mechanics and molecular simulations to the study of hydration of DNA bases. Honig's group further develops ideas of bridging 'microscopic' and macroscopic surface tensions. B.K. Lee addresses problems of the standard state in the description of hydration processes, of the entropy–enthalpy compensation and the role (or rather its absence) of hydrogen bonds in hydrophobicity. R. Levy detects nonlinearities in the dielectric response studies with molecular mechanics. Makhatadze and Privalov continue to apply their ideas on the role of hydration in protein folding to an expanded set of proteins studied by them calorimetrically. Y. Marcus reviews a wide range of experimental data on hydration of a wide variety of ions and attempts to describe it with an empirical model. K.P. Murphy reviews the issue of convergence temperatures and introduces a controversial interpretation of the origin of hydration entropies of alcohols. Nauchitel and Somorjai revisit derivation of hydration parameters from distributions of side chains in globular proteins and appplications of such parameters to antigen–antibody recognition. M. Paulaitis presents further developments of methods to extract hydration entropies from the results of molecular simulations. Perkyns and Pettitt review recent developments in the integral equation techniques and their applications to ionic solutions. L. Pratt et al. review studies of potentials of mean force and suggest some new approaches to their study. A. Rashin with coworkers review main features of thermodynamics of hydration as revealed by the continuum approach, analyze the ability of this approach to provide a quantitative theory, and present its combination with quantum mechanical density-functional theory for studies of hydration. A. Schmidt analyses volume effects in transfer to model liquids. A scrutinizing discussion by the participants binds these distinct studies into a coherent (and often full of conflicts) view of the field.

We hope that the Special Issue "Thermodynamics of Hydration" achieved its goal and would entice its readers to actively participate in further development of this exciting field of knowledge.

The Guest Editor of the Special Issue
Dr. Alexander A. Rashin
10 March 1994.