

## PREFACE

This special issue of *Croatica Chemica Acta* contains the papers presented at the INTERNATIONAL SYMPOSIUM ON APPLICATIONS OF MATHEMATICAL CONCEPTS TO CHEMISTRY, held in Dubrovnik, Croatia, from September 2 to September 5, 1985. The Symposium was organized under the sponsorship of *The Union of Pure and Applied Chemistry* in conjunction with the *Union of Chemical Societies of Yugoslavia*, the *Croatian Chemical Society*, and the *Department of Physical Chemistry of the Rugjer Bošković Institute in Zagreb*.

The Scientific Committee included the following scientists, active in both mathematical and computational chemistry: N. L. Allinger (Athens, GA, USA), F. DeLos DeTar (Tallahassee, FL, USA), F. E. Harris (Salt Lake City, UT, USA), R. B. King (Athens, GA, USA), Z. B. Maksić (Zagreb, Croatia, Yugoslavia), P. G. Mezey (Saskatoon, Saskatchewan, Canada), O. E. Polansky (Mülheim/Ruhr, BRD), L. J. Schaad (Nashville, TN, USA), and N. Trinajstić (Zagreb, Croatia, Yugoslavia).

The Organizing Committee consisted of the following people from Zagreb: S. Bosanac, T. Cvitaš, A. Graovac, K. Kovačević, Z. Majerski, Z. B. Maksić, Z. Meić, N. Nekić, Lj. Ruščić, A. Sabljčić, B. Špoljar, N. Trinajstić and T. Živković.

Financial support was given by the *Union of Associations for Scientific Research of Yugoslav Republics and Autonomous Provinces*, *Brüker Analytische Messtechnik, GmbH, Karlsruhe*, and the *Department of Physical Chemistry, The Rugjer Bošković Institute, Zagreb*.

Not so very long ago, several researchers from different countries, working in various fields of theoretical chemistry, suggested that an international symposium on some aspects of Mathematical Chemistry should be organized. These included Professor B. M. Gimarc (Columbia, SC, USA), Professor M. Randić (Ames), Professor D. J. Klein (Galveston), Dr. R. B. Mallion (Canterbury), Dr. D. Bonchev (Burgas), Professor P. G. Mezey (Saskatoon), Professor J. V. Knop (Düsseldorf), Dr. P. Křivka (Pardubice), Professor B. A. Hess, Jr. (Nashville), Professor A. T. Balaban (Bucharest). The suggestion specifically proposed the Theoretical Chemistry Group at the Rugjer Bošković Institute in Zagreb as organizer, primarily because of our past active role in developing and promoting Mathematical Chemistry in general, and Chemical Graph Theory in particular. We accepted the responsibility, both as an honour and a privilege. We are specially pleased that the long standing tradition of Mathematical Chemistry in this country, and in Croatia in particular, has been recognized in this way. Thus, this first symposium dealing exclusively with topics that constitute Mathematical Chemistry has been organized by our Group with great fervour and enthusiasm.

Dubrovnik was chosen as the site of the Symposium because it is one of the most interesting Croatian cities, with an outstanding historical, cultural,

and scientific heritage. The famous Croatian scientist Rugjer Bošković, Fellow of the Royal Society (London), Professor of Mathematics at Collegium Romanum in Rome, and found of the Observatory at Brera, was born there (May 18, 1711). Furthermore, Dubrovnik, known for its mild Mediterranean climate, is a frequent site of scientific gatherings, and is easily accessible by land, sea and air.

The International Symposium on the Applications of Mathematical Concepts to Chemistry was held in hotel »Libertas« in Dubrovnik and was attended by 128 participants: 69 from 20 countries and 59 from all Yugoslav Republics and Autonomous provinces, except Montenegro and Vojvodina. The Symposium brought together mathematical and computational chemists, computer chemists, theoretical chemists, mathematically and theoretically minded experimental chemists, mathematical physicists and mathematicians, for discussions on the status of mathematical chemistry, its perspectives, and its influence upon various aspects of chemistry.

The last day of the Symposium was dedicated to the memory of the late Professor Andrej Ažman (Celje 1937 — Ljubljana 1980) who, in his time, was one of the leading chemical theoreticians in Yugoslavia and an inspiring supporter of mathematical chemistry.

Last but not least, important preliminary steps were made during the Symposium to establish an International Society of Mathematical Chemistry. The following scientists were elected to organize the structure of the Society: D. Bonchev (Burgas), H. Hosoya (Tokyo), R. B. King (Athens, GA), P. G. Mezey (Saskatoon), O. E. Polansky (Mülheim/Ruhr), M. Randić (Ames) as acting president, and D. H. Rouvray (Athens, GA) as acting secretary. There was also vigorous discussion on starting a new journal whose aim would be to cover all aspects of mathematical chemistry.

We hope that the combination of the exciting science, beautiful scenery, warm weather and hospitality of the local people made the Symposium a memorable experience for all participants.

The lectures and posters covered a significant part of the broad spectrum of problems in mathematical chemistry and its interactions with other areas of chemistry. The Symposium also revealed the permanent need for mathematics in all branches of chemistry.

A gratifying observation was that in most of the presented papers on mathematical approaches to chemistry, the focus was on considerations of chemistry rather than just on mathematics. Besides, it became evident that mathematical chemistry will continue to grow as a part of theoretical chemistry; other overlapping, but distinguishable, parts include the quantum chemistry, statistical mechanics and computational chemistry. Supportive of this statement are the announcements of a Symposium on Computational and Mathematical Chemistry (June 1—4, 1986, Saskatoon, Saskatchewan, Canada; Organizer: Prof. P. G. Mezey) and an International Conference on Graph Theory and Topology in Chemistry (March 8—13, 1987, Athens, Georgia, USA; Organizer: Prof. R. B. King and D. D. H. Rouvray). In addition, one of the topics planned for the 26th Sanibel Symposium (March 10—15, 1986, Marine-land, Florida, USA; Organizer: Prof. P. O. Löwdin) is graph theory and chemical applications.

The invited papers presented at the Symposium will appear in the book *Mathematics and Computational Concepts in Chemistry* (edited by N. Trinajstić), to be published by Ellis Horwood, Ltd. (Chichester, England).

In this issue of *Croatica Chemica Acta* we were able to publish only those papers presented at the Symposium, orally or on posters, which have been received before the agreed deadline. In addition, each paper was refereed by two independent referees, internationally recognized experts in the field of mathematical (and computational) chemistry, so that only papers with favourable reports were accepted for publication.

On behalf of the *Scientific Committee* and the *Organizing Committee* we would like to express our gratitude to the listed sponsors and organizations for their help in the preparation of the Symposium and for financial help. Finally, we thank Dr. Matko Orhanović (The Rugjer Bošković Institute, Zagreb), for showing his understanding of our problems and for his help in every way.

Zagreb, December 1985.

NENAD TRINAJSTIĆ