

PREFACE

Discussions in Nashville with Professors B. A. Hess, Jr. and L. J. Schaad in early spring of 1980 about the direction of the development of Theoretical Organic Chemistry led to the idea to organize *The International Symposium on Theoretical Organic Chemistry*. We decided that the aim of the Symposium should be to attempt to bring together theoretical chemists and theoretically minded experimental chemists for lectures and discussions about the present status of Theoretical Organic Chemistry and about its influence on, and interactions with, Preparative Organic Chemistry. Many colleagues in Japan, U.S.S.R., Germany, Hungary, U.S.A., China, France, Czechoslovakia, Rumania, Bulgaria, England, etc. enthusiastically reacted to this idea and we began in autumn 1980 with the organisation of The International Symposium on Theoretical Organic Chemistry.

The Symposium was organized under the sponsorship of The International Union of Pure and Applied Chemistry in association with The Union of Chemical Societies of Yugoslavia, Croatian Chemical Society, and The Department of Physical Chemistry, The Rugjer Bošković Institute, Zagreb.

The *Scientific Committee* was made up of the following scientists: N. L. Allinger (Athens, Georgia), R. Gleiter (Heidelberg), K. N. Houk (Pittsburgh), J. Michl (Salt Lake City), D. E. Sunko (Zagreb), and N. Trinajstić (Zagreb). The members of The *Organizing Committee* were A. Graovac (Zagreb), P. Ilić (Sarajevo), L. Klasinc (Zagreb), N. Nekić (Department of Physical Chemistry, The Rudjer Bošković Institute, Zagreb).

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1982 was selected for the Symposium year because it coincided with the 30th anniversary of theoretical (organic) chemistry in Zagreb and Croatia. In late spring of 1952 Professor Milan Randić (presently at The Department of Mathematics and Computer Science, Drake University, Des Moines, Iowa, U.S.A.) completed his diploma work on the electronic structure of benzene under the guidance of Professor Ivan Supek (a former student of Werner Heisenberg). After obtaining his Ph. D. degree at Cambridge under Professor Norman Sheppard, Professor Randić returned to Zagreb and founded the Theoretical Chemistry Group at the Rugjer Bošković Institute. Thus, Professor Randić was the first scientist doing research in theoretical (organic) chemistry in Croatia.

The International Symposium on Theoretical Organic Chemistry was held in hotel »Libertas«, Dubrovnik (Croatia) from August 30 to September 3, 1982. It was attended by 133 participants: 82 from 23 countries and 51 from all Yugoslav Republics and Autonomous Districts. The combination of exciting chemistry, beautiful scenery and warm weather made the meeting a memorable experience for all participants.

There were quite a few presentations at the Symposium: 26 invited lectures (24 given orally and 2 on posters), 18 contributed lectures and 46 posters. They covered a variety of topics: 'exact' and approximate calculations, applications of the qualitative theories of organic chemistry such as PMO, HMO, maximum overlap method, or topological methods, construction of potential energy surfaces, theories of aromaticity, predictions of new compounds, predictions of properties of molecules and their reactivities, reaction mechanisms, developments of new structurally — based organic nomenclature, aromatic photosubstitutions, lithium synthetic reagents, enumeration of isomeric structures, the use of various spectroscopy techniques in organic chemistry, etc.

The invited papers presented at the Symposium will appear in a special issue of *Pure and Applied Chemistry*, the official journal of The Union of Pure and Applied Chemistry. In this issue of *Croatica Chemica Acta* we could publish only those contributed papers presented at the Symposium, orally or on posters, which had been received before the agreed dead — line. In addition, each paper was refereed by two independent referees, internationally recognized as experts in the field of (theoretical) organic chemistry, so that only papers with favourable reports were accepted for publication. For practical reasons (in order to avoid one large volume of the Journal), the accepted papers are printed in two parts. **Part I** contains papers with a strong experimental background, while more formal papers appear in **Part II**.

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 Symposium and for financial support.

Finally we thank Dipl. Ing. Stjepan Lisjak (INA — Petroleum Industry, Zagreb), Dr. Franjo Kajfež (Podravka — Belupo, Koprivnica), and Dr. Matko Orhanović, (The Rugjer Bošković Institute, Zagreb), for showing their understanding for our problems and for their help in every way.

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