



Professor Dušan Hadži – 90 years old

There are not many people in the modern scientific world that have substantially contributed to several branches of chemical research, such as quantum chemistry, artificial intelligence and chemometrics, materials- and structure characterization and pharmaceutical active ingredients. The scientific research of academician professor doctor Dušan Hadži has been scientifically highly productive and his discoveries undoubtedly represent such an achievement.

His scientific career has been long, rich, and extensive, ranging from theoretical studies and explanations of hydrogen bond, through the establishment of laboratories with modern instruments and employing top researchers, to the practical solutions for human health welfare and environmental benefits.

He was born on August 26, 1921 in Ljubljana. He obtained his B. Sc. degree from the Chemistry Section of the Faculty of Philosophy and received his Ph. D. from the Faculty of Natural and Mathematical Sciences at the University of Ljubljana.

After his employment in 1948 at the Institute of Chemistry of the Slovenian Academy of Sciences and Art his first research task were the explanation of structure and properties of coals and the theoretical explanation of coke formation from young coals containing high levels of sulfur. It was at that time that infrared spectroscopy be-

gun to emerge as one of the most important techniques for the study of macromolecular structures. Professor Maks Samec, then the director of already independent Institute of Chemistry, realized the need for acquiring new ideas and knowledge from already established sources in order to successfully introduce new modern research techniques. Following this suggestion, Professor Hadži went to the University of Cambridge, England, for a period from 1950–1951 to further specialize in the field of infrared spectroscopy. After earning his Ph. D. in 1953 he managed to introduce the first infrared spectrometer in Ljubljana that opened the way for the continuation of theoretical research of the studies of hydrogen bonds in organic molecules, with an emphasis on short hydrogen bonds in OH groups. Professor Hadži published a classification related to this field that has become one of the most cited in the world and has been in use ever since.

The ideas of the nature of hydrogen bond spread throughout the scientific world. The research continued by the use of a variety of other techniques as X-ray diffraction, inelastic neutron scattering, incoherent inelastic neutron scattering, far infrared spectroscopy, Raman spectroscopy, nuclear magnetic resonance and quadrupole nuclear magnetic resonance. These techniques had slowly established themselves in Slovenian research area and, by a substantial engagement of Professor Hadži, enabled more detailed structure investigations and also became research tools for highly-specialized researchers.

As a natural consequence of using different investigative techniques there emerged an idea on the possible use of artificial intelligence in chemical research. The application of these ideas has through the years evolved into independent chemometric investigations.

A new challenge in the scientific career of Professor Hadži was the development of quantum methods for the study of medium-size molecules and the role of hydrogen bonds in biological processes. The main areas studied were the mechanisms of enzyme reactions and molecular recognition. The important reactions studied were proton transfer and hydrogen bond orientation.

By the end of 1980s Professor Hadži initiated and started the investigations in the field of peptide-based active ingredients. The research included specialists from Lek Pharmaceutical Company, Faculty of Pharmacy, Institute of Immunology and Microbiology and Ruđer Bošković Institute from Zagreb, Croatia. The research was of great importance to the pharmaceutical industry and was focused on interaction of active ingredients or appropriate model molecules with phospholipids. He solved several challenging problems by the ingenious use of infrared spectroscopy and model calculations.

Lately, there had emerged a renewed interest in the role of strong hydrogen bonds in the energetics of enzyme reactions and Professor Hadži returned once again to the studies of this topic. With the fruitful collaboration of numerous partners from Europe and the U. S. A. he decided on quantum characterization method. He succeeded in describing the proton dynamics and established the correlations among various parameters on the basis of the increase of interaction degree and the changes of proton center-of-gravity.

The scientific work of Professor Hadži was always present in the international scientific arena that he frequently succeeded in transferring it to the home ground. As early as 1957 he organized the conference on hydrogen bond, the first after the World War II, that brought together numerous eminent scientists from the West and East, among them L. Pauling and G. Pimentel (U.S.A.), J. D. Bernal and C. A. Coulson (Great Britain), M Eigen (Germany) and M. A. Volkenstein and N. D. Sokolov (then Soviet Union). He organized, together with J. Zupan, the 2nd international conference on the use of computers in chemical research and education in 1973. In 1986 he was the organizer of the 6th international symposium on quantitative relationships between the structure and activity that was

held in Portorož, Slovenia. He actively presented his work and that of his collaborators, mostly as invited lectures, at international conferences and universities throughout the world.

He shared his knowledge, scientific creativity and excellence and perseverance in work with his junior colleagues and assistants which have, as a result, evolved into eminent independent researchers, scientists and educators.

Professor Hadži's whole scientific career has been mostly affiliated with the Institute of Chemistry (now National Institute of Chemistry), where he was also a director. His contributions also helped the Institute to maintain the status of a research institution which, together with top, young researchers faces the ever-arising new challenges. He also worked at the Faculty of Natural Sciences and Technology at the University of Ljubljana and at Lek Pharmaceutical Company.

In the course of his scientific career of over 60 years, Professor Hadži published more than 280 original scientific papers and 9 chapters in monographs, authored 4 books and edited the proceedings of three international congresses. The impact of his works has been reflected in more than 3.000 citations. He also published several critical contributions on the position and status of science in our society as well as other important themes regarding the civil society.

He was the president of the Slovenian Chemical Society from 1974 to 1986 and currently acts as the Society's Honorary President. He also performed numerous important duties in the research authorities of the Republic of Slovenia.

Professor Hadži received numerous decorations, awards and commendations for his highly praised scientific work from the State and from professional societies. He has been a regular member of the Slovenian Academy of Sciences and Arts and an external or corresponding member of several foreign Academies. He also received an honorary doctorate from the University of Uppsala, Sweden. He has been an honorary member of many professional associations and societies.

On the occasion of Professor Hadži's important anniversary, we all wish him good health, continuing optimistic spirit and further success with studying hydrogen bonds. All the best!

Venčeslav Kaučič
President, Slovenian Chemical Society