

Nenad Trinajstić – *curriculum vitae*

Professor Nenad Trinajstić was born on January 26, 1936 in Zagreb, where he finished the seven-year elementary school (1951; at that time he already started doing simple chemical experiments, some of which were not so simple and ended in violent explosions) and high school (1956). He graduated from the Department of Chemical Technology of the Technological Faculty in Zagreb in 1960 (his degree-thesis supervisor was Professor Ivan Filipović of Haldenthal (1911–1998)). The degree-thesis was entitled *Influence of pH on the Half-wave Potential of Bismuth in Solutions of Sodium Acetate and Acetic Acid* (»Utjecaj pH na poluvalni potencijal bizmuta u otopinama natrijeva acetata i octene kiseline«, University of Zagreb, 1960). He won his master's degree in 1966; his master-thesis supervisor was Professor Milan Randić. The title of his M.Sc. thesis was *The Method of Maximum Overlap and Its Application to Calculation of Hybrids in Some Methyl-substituted Cyclopropanes* (»Metoda maksimalnoga prekrivanja i primjena na izračuna-

vanje hibrida nekih metil-supstituiranih ciklopropana«, University of Zagreb, 1966). In his M.Sc. thesis N. Trinajstić applied the Coulson-Moffitt maximum overlap method, in a modified form, to all possible methyl-sub-



Professor Ivan Filipović of Haldenthal, under whose guidance Nenad Trinajstić did research in polarography for his degree thesis, delivering a speech on the occasion of the 70th anniversary of Chemical Technology Studies at the Croatian National Theatre (Zagreb, October 20, 1989).



Nenad Trinajstić and his younger brother Ivan just after graduation on November 12, 1960.

stituted cyclopropanes. He got his doctor's degree from the Faculty of Science and Mathematics in 1967. His doctoral thesis, entitled *Electronic Structure of Some Polyatomic Molecules* (»Elektronska struktura nekih poliatomnih molekula«, University of Zagreb, 1967), was the first Croatian dissertation in quantum chemistry. Research on which his Ph.D. thesis was based was carried out under the supervision of Professor John N. Murrell, FRS, at the Universities of Sheffield (1964–1965) and Sussex (1965–1966). In his Ph.D. thesis he reported the use of the Pariser-Parr-Pople SCF MO method to interpret the UV/VIS spectra of alternant hydrocarbon anions and cations and several original criteria for obtaining localized orbitals. Nenad Trinajstić was a Robert A. Welch post-doctoral research fellow in the Department of Chemistry, University of Texas in Austin (1968–1970), where he work-

ed with Professor Michael M. J. Dewar, FRS (1918–1997) on studying the structure and properties of various large organic molecules by semiempirical SCF π -MO and MINDO methods using original parameterization.

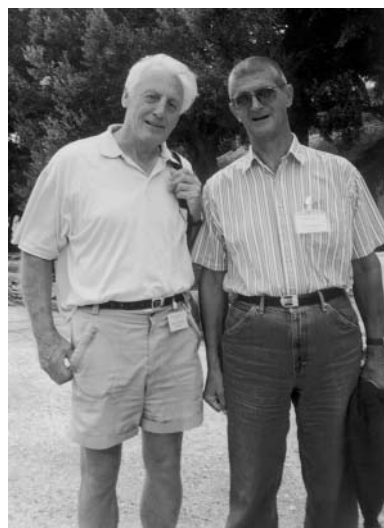
After receiving his B.Chem.Techn. degree, he was employed by the Pliva Research Institute (1960–1961), wherefrom he moved to the Rugjer Bošković Institute (RBI) in early 1962, where he spent all his working life. He was for many years head of the Theoretical Chemistry Group in the Department of Physical Chemistry and after the RBI was reorganized, he served as head of the Physical Chemistry Division (1997–2001). He retired at the end of 2001. His advancement in research positions in RBI proceeded as follows: research assistant (1962–1967), research scientist (1967–1971), associate research professor (1971–1977), full research professor (1977; reelected 1998), and in teaching positions in the Faculty of Science and Mathematics: assistant professor (1970–1973), associate professor (1973–1977) and full professor (1977–



Professor Milan Randić and Nenad Trinajstić in St. Augustine, Florida (the City of St. Augustine was established in 1565 and is America's oldest city) at the monument of Father Francisco Lopez de Mendoza Grajales, the first Catholic priest in North America. The monument is the work of the famous Croatian sculptor Ivan Meštrović (1883–1962). The photo was taken on March 4, 1997 when Randić and Trinajstić attended the 37th Sanibel Symposium (St. Augustine: March 1–7, 1997).

1998), and from 1998 titular full professor. Fifteen degree theses, 12 master theses and 20 doctoral theses have been made under his supervision.

He was awarded the City of Zagreb Award in 1972, the state award for science »Rugjer Bošković« in 1982, and the Mid-America State Universities Association (MASUA) Distinguished Foreign Scholar award in 1986. On the occasion of his 60th birthday, his former students, colleagues and friends from Zagreb and abroad, in conjunction with the Croatian Chemical Society, Faculty of Chemical Engineering and Technology and Matrix Croatica (Matica hrvatska), organized a day-symposium on October 25, 1996.



Professor John N. Murrell FRS and Nenad Trinajstić at the Brijuni Conference 2002 (Brijuni, Croatia: August 26–30, 2002).



Professor Michael J. S. Dewar FRS and Nenad Trinajstić at the 28th Sanibel Symposium (Marineland, FL, USA: March 12–19, 1988).



All theoretical chemists, except for Milan Randić, who were working on resonance energy during the 1970s met in Jerusalem in 1981 at the Fourth International Symposium on the Chemistry of Novel Aromatic Compounds (ISNA 4, August 30 – September 4, 1981). From left to right: Nenad Trinajstić, Lawrence Schaad, B. Andy Hess, Ivan Gutman, William C. Herndon, Roger B. Mallion and Jun-ichi Aihara.

A special issue (guest editors D. J. Klein and S. Nikolić) of *Internet Electronic Journal of Molecular Design* (<http://www.biochempress.com>) was also dedicated to Professor Trinajstić on the occasion of his 65th birthday.

Professor Nenad Trinajstić has served and is serving on editorial boards of several journals: *Croatica Chemica Acta* (1967–1994), *Journal of Molecular Structure-Theochem* (1985–1995), *Journal of Mathematical Chemistry* (1986–1989, and again since 1994), *Symmetry* (1989–1990), *Computers and Chemistry* (1989–2002), *MATCH-Communications in Mathematical and in Computer Chemistry* (since 1997), *SAR & QSAR in Environmental Research* (since 1999), *Gazophylacium* (since 2000), *Computational Biology and Chemistry* (since 2003). He was co-editor-in-chief of *Journal of Mathematical Chemistry* (1990–1993) and is currently editor-in-chief of *Croatica Chemica Acta* (since 1994) and *Prirodoslovlje* (since 2001). He also sits on advisory boards of *Bulletin of the Chemists and Technologists of Macedonia* (since 1995) and *Polymers* (since 1998). He is a member of *Matrix Croatica* – the Central Croatian Cultural and Publishing Society established in 1842 (since 1955) and *Croatian Chemical Society* established in 1926 (since 1960), *Croatian PEN Club* (since 1987), *Brethren of Croatian Dragon* – an old Croatian fraternal society established in 1408 as the *Knights' Order of Dragon* (since 1991), and the *Croatian Academy of Sciences and Arts* established in 1861 (since 1992), etc.

Professor Trinajstić's research interests lie in the fields of quantum chemistry, mathematical chemistry, computer

chemistry, history of chemistry and especially in the history of Croatian chemistry. Two topics prevail in quantum chemistry: development of the semi-empirical molecular-orbital theory applicable to large (heterocyclic) molecules and the setting up of a model, named the conjugated circuits model, on a firm quantum-mechanical basis, its parameterization and application to different classes of conjugated molecules and fullerenes. In the field of mathematical chemistry, he works on the development and application of graph theory and topology to chemistry – the most interesting result being the formulation of topological resonance energy as a measure of aromaticity of conjugated systems. He was also involved in the development of molecular descriptors known as topological indices (Zagreb indices and their modifications, Harary index, various distance indices, detour index, etc.) and in the development of quantitative relations between the structure, properties and activities of organic molecules and biomolecules (e.g., the CROMRsel method). His research in computer chemistry involves the development of algorithms for characterization, generation and enumeration of chemical structures that can be used to generate (virtual) combinatorial libraries. His most valuable results in this field are the development of algorithms for constructive enumeration of acyclic structures (the N-tuple code) and certain classes of polycyclic structures (the DAST code). His research topics in the history of chemistry include the events and persons relevant to Croatian chemistry.

His contributions in the fields of chemical graph theory and the graph-based computer chemistry made him well known in scientific literature as one of the pioneers of these branches of mathematical chemistry. He wrote the first single-author book on chemical graph theory (*Chemical Graph Theory*, CRC Press, Boca Raton, 1983, second edition 1992, third edition in preparation). Professor Trinajstić is one of the most cited Croatian chemists.

He has published more than 500 research papers, about 150 technical papers, more than 250 book reviews, biog-

raphies of Croatian chemists, popular-science papers, and 11 books. His first book *Molecular Orbitals in Chemistry* was published in 1974 by Školska knjiga in the series *Contemporary Chemistry* (which he initiated with Krešimir Humski (1939–1997)). This was the first book to deal with theoretical chemistry in the Croatian language. His most recent (eleventh) book *100 Croatian Chemists* (Školska knjiga, Zagreb) was published in 2002.

Sonja Nikolić