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Scientific Journey of Zvonimir Maksić

It is a difficult task to write on the scientific career of Zvonimir Maksić, because it is long, rich and multifaceted reflecting a wide spectrum of his interests ranging from molecular physics through chemistry to the molecular biology and (ortho)molecular medicine. He went a long way of a theoretical chemist who started with the pencil and paper calculations by using mechanical calculators, over semiempirical calculations on small computers based on perforated ribbons and boxes of punched cards, to be dragged to the computer centres, and who has heavily used the modern *ab initio* computation methods in some of the largest supercomputing facilities in the world *via* internet connections in the last two decades. It is a story of a researcher in a remote country with limited resources, where grave problems in research could be surmounted only by creativity and very hard work. A long list of the published papers witnesses his persistence and devotion to science. Although we know a lot about his research, particularly since we had a chance to work with him over many years, there were some gaps in our knowledge. In order to bridge them, we had to make several interviews with Professor Maksić. This was a lot of fun, since he did not only provide required information and materials, but shared also with us reminiscences about many remarkable scientists including Ivan Supek, Božo Težak, Linus Pauling and Rolf Gleiter, who influenced his life and career the most, albeit in different ways. We are aware of the fact that biography condensed in a few pages must be incomplete. Nevertheless, we believe and hope that the most important moments are well described.

The Beginnings

Zvonimir Maksić was born in Bitola (Republic of Macedonia) on September 11, 1938. He attended the elementary and high school in Zagreb. As a child he liked to read Shakespeare's dramas and Jules Verne's science fiction novels. However, two books were decisive. The first was biography of Louis Pasteur. He was impressed by a number of discoveries made by a single man. The other was Ivan Supek's "From Antique Philosophy to the Modern Theory of Atoms". That book was a revelation and he described it like an entrance to the wonderland of atoms and molecules. Since that moment he knew that his profession would be science. His interests in the high school were mainly focused to physics and chemistry. Most of the time, however, he spent studying and playing chess. The game of kings was enchanting with its logical structure, elegance and artistic pleasure offered by the chess combinations. In a way, this was a preparation for scientific career without knowing it.

After graduation at high school, he started to make plans for the future. His father, who was a professor of geophysics and meteorology at the University of Zagreb, warned him that academia can offer a very modest living standard, which is "compensated" by many obstacles, but he would not listen. Striving to learn what atoms are doing in molecules and how tiny molecules affect properties of large objects, *i.e.* molecular materials, he enrolled chemical physics just introduced at the Faculty of Science of the University of Zagreb. This curriculum was dismantled after just one year as "too difficult"! This twist of fate turned to be a useful one, because he switched to theoretical physics, which was rather strong in Zagreb. It was led by Ivan Supek, who was a member of Heisenberg's seminar in Leipzig before the Second World War and who obtained his Ph.D. working with Friedrich Hund. Ivan Supek inaugurated Leipzig's theoretical physics curriculum in Zagreb. Zvonimir Maksić took a large number of courses in mathematics and quantum theory, which proved useful in his later work in quantum chemistry. After receiving B.Sc. degree he accepted position of research assistant at Ruđer Bošković Institute (RBI) in 1962. The RBI was founded by Ivan Supek in 1950 and became the most important institute for natural sciences in Croatia. Zvonimir Maksić started to work with Milan Randić, who came back from England (Cambridge), where he received Ph.D. in molecular spectroscopy. The start–up equipment was a small mechanical desk calculator,

which has been making terrible noise when used, thus causing protests of the readers in the next–room library. In retrospect, it was a blessing, because one was forced to think very carefully what to do and why to do it before starting calculations. Among a couple of offered themes, he selected to work on hybridization of atomic orbitals, which proved to be a fortunate choice.

The Model Building

Hybridization was discovered by Linus Pauling eighty years ago in his two milestone papers[1] and discussed *in extenso* in the book considered as a bible of chemistry of the 20th century.[2] This seminal concept was introduced in order to describe the local symmetry of an atom defined by its immediate chemical environment. Following footsteps of Charles A. Coulson,[3] Randić and Maksić used the criterion of maximum overlapping and determined hybridization in some highly strained hydrocarbons, which were at the focus of interest in organic chemistry.[4,5] The work on bicyclo[1.1.0]butane was particularly interesting, because the twisted chemical bond was found for the first time.[5] Unfortunately, Zvonimir Maksić was drafted to serve the army for a year. As a Croat in strongly pro–Serbian Yugoslav Army, he had a very hard time. After a year of thorough brainwashing he returned to the RBI and was able to continue work at the end of a longer convalescence period. He finished up Ph.D. thesis under a guidance of M. Randić in 1968. Around that time he met a young physical organic chemist Mirjana Eckert. Soon they started to work together at the Institute and their own home. Afterwards, they went for postdoctoral studies, first at the University of Tennessee in Knoxville (with John Bloor) in 1970–1971 and then at the University of Texas at Austin (with Michael J. S. Dewar) in 1972–1973. Returning to Zagreb and the RBI, he took position of a research associate in 1973 and a position of a part time associate professor at his *Alma Mater*, the Faculty of Science of the University of Zagreb. He has held research and teaching positions at both institutions ever since, until recent retirement.

In Zagreb he tried first to round up the work on hybridization. The slightly modified Muller–Pritchard and Bernstein formulae for calculations of the J(C–H) and J(C–C) spin–spin coupling constants of directly bonded nuclei, based on variable hybrid orbital (HO) model were in very good accordance with experiments[6,7] possessing a high predictive power. The same approach was extended to some other nuclei.[8,9] An important refinement was introduced by the Iterative Maximum Overlap Method,[10,11] which made possible optimization of structural parameters, *i.e.* it gave both the shape and the size of molecules. Interestingly, the HO model, designed for description of local covalent bonds, proved very useful in interpreting global molecular properties like geometries,[10–12] heats of formation and hydrogenation,[13] angular strain energies,[14] isopycnic deformation contours of the electron density distributions,[15] and even UV spectral transitions in highly strained hydrocarbons,[16] as well as some of the magnetic properties.[17] At the same time, HOs were useful for qualitative and semiquantitative interpretation of local bond properties in addition to the already mentioned spin–spin coupling of directly bonded atoms: the intrinsic bond energies,[18] the isolated stretching frequencies of C–H bonds,[19] symmetric and asymmetric stretching frequencies,[20] the C–H, C–C and C=C stretching force constants[21,22] and C–H bond acidity.[23] Interestingly, the hybridization has also a strong influence on the C–H proton isotropic hyperfine coupling constants in planar radicals.[24] Last and perhaps the most important, several new inter–relations between various observables were derived (*via* hybrids' s–character and the overlapping integrals), which have not been known earlier.[22] Despite the fact that the s–characters cannot be measured directly and defined in a unique way, they affect a large number of molecular properties. For that reason the hybridization was termed a pseudo-observable.[22]

The hybridization model was successful, because it inherently included two most fundamental facets of covalent bonding: (1) local symmetry and the spatial arrangement of covalent bonds, and (2) the bond strength embodied in overlapping. Additionally, polarization of the HOs in particular directions in space minimized its presence in others, thus diminishing Pauli repulsion between electron pairs. The HOs describe also the electron correlation (see later). The efficacy of the HO model gives rise to the idea that atoms are perturbed in molecules, but retain their identity. This means that molecules are not structureless droplets of the nuclei and electrons, which is gratifying. Instead, they have structured arrangements of constituent atoms, which are (slightly) modified compared to their free–state features. This memory effect is reflected in a wide variety of molecular properties as evidenced by a number of atomic additivity rules. The performance of the latter were conclusively illustrated by the second moments of the electron density distributions[25] and the related diamagnetic susceptibilities (Langevin's terms).[23,26–28] By using these additivity formulae, Professor Maksić was able to interpret a 100 years old Pascal's empirical rule governing behaviour of the temperature independent magnetic susceptibility of molecules.[29] It turned out that Pascal's constants were weighted free–atom magnetic susceptibilities.[30,31] This was the first theoretical rationalization of Pascal's empirical scheme, which was of importance, because this scheme has had numerous applications in reproducing the experimental data.[32] It should be mentioned in passing that the averaged dia-

magnetic shielding of the NMR shift also exhibits atomic additivity.[31,33–37]

A strong support to the picture of atoms in molecules came from the experimental X–ray photoelectron spectroscopy (ESCA).[38] It appears that ejection of the local inner-shell electrons of particular atoms provides a wealth of information on the electronic structure of molecules. Although the core-electrons are inert in the chemical bonds formation, they are keen observers of the changes occurring in their environment. There is plethora of papers and data on ESCA theory, applications and experiments. Kai Siegbahn received for this work the Nobel Prize in Physics in 1981. A small contribution to the interpretation of ESCA spectra was provided by calculations, which have shown that the best atomic monopole electrostatic potentials, needed for that purpose, could be obtained by the self–consistent charge MO method.[39,40] A good agreement with experiment was attained for a wide variety of compounds including nucleic acid bases[41] and some other biologically important molecules.[42] A conceptually crucial outcome of the ESCA work is that the core–ionization energies taken together with Auger kinetic energies offer the best estimates of otherwise elusive atomic charges in molecules, which can not be defined in a unique way. A comprehensive discussion of this topic can be found in reference 43.

The work on perturbed atoms in chemical environments has led to a model of modified Atoms in Molecule (MAM).[31,44] The changes in atoms caused by chemical bonding are characterized by descriptors like degree of hybridization, by atomic electric multipoles etc. The MAM model gives simple, transparent and intuitively appealing rationalization of molecular properties at qualitative or semiquantitative level based on the atomic, bond or group additivity rules. It explains fingerprints left by atoms or their functional groups in the experimentally measured or accurately calculated observables. The MAM model also describes the substituent effects of particular atoms on the main body of the molecule and its features. This model is approximate version of the rigorous quantum theory of atoms in molecules developed by Bader and coworkers.[45] Bader's virial atoms give each observable as an exact sum of atomic contributions. The problem is that construction of surfaces of the virial atoms in molecule is tedious and computationally very demanding, which hinders applications in very large systems.

An interesting support to the modified atoms picture was obtained afterwards by considering the electron correlation energies in molecules. It was shown that the correlation energy in Lewis molecules is given by a sum of atomic terms to a good accuracy, if the canonical hybridization states of atoms are taken into account.[46,47] A convincing evidence has been presented in an important *tour de force* paper that the DFT–B3LYP correlation energy can be obtained by simple scaling of the corresponding energies computed by the *ab initio* wavefunction methods.[48] This conjecture straightforwardly follows from the additivity rule. The relevance of this result stems from the fact that the correlation energy in the density functional theory (DFT) is defined implicitly in an *ad hoc* manner. It is also remarkable that the electron correlation of Lewis molecules can be calculated on the back of a postcard.[46–48] An even more accurate additivity scheme was developed later along the same lines by Klaus Ruedenberg.[49] Surprisingly, it turned out that the nondynamical correlation of the π–electrons in polyenes is also additive, but exhibits interesting counterintuitive nonadditivities in anti/aromatic systems.[50,51] As a footnote, it should be mentioned that the zero point vibration energies follow simple atomic additivity rule, albeit only approximately.[52] The bottom line of all these investigations is that the concept of modified atoms in the molecules has a high interpretive value.

The Vitamin C Episode

Zvonimir Maksić had intensive correspondence with Linus Pauling lasting for many years since the early work on the hybridization model. Pauling was always responsive and ready to give advice. His suggestions and encouragement were highly stimulating and helpful. Under Pauling's influence, Professor Maksić started to work on the electronic structure of vitamin C and its derivatives. The focus was on the ascorbic acid (AA) tautomers, their radicals, anions and the solvent effects in water.[53–59] The final goal was elucidation of the mechanism of the AA biochemical reactivity, which was not and still is not well understood. Unfortunately, the semiempirical methods available at that time were not accurate enough for that purpose. Regretfully enough, this work was never resumed by efficient *ab initio* methods at disposal nowadays. Theoretical considerations were combined by experimental investigations *in vitro* and *in vivo* in collaboration with Krešimir Pavelić at RBI and Constance Tsao, senior researcher at the "Linus Pauling Institute of Science and Medicine" in Palo Alto, USA. It was found that vitamin C induces apoptosis in human tumor cells,[60] and that its derivatives suppress the malignant growth in mouse melanoma cells[61] as well as in leukaemia cell line *in vitro*.[62] The results of investigations carried out at RBI are summarized in a short review article.[63] Although these investigations did not lead to a new treatment, it was shown beyond any doubt that the ascorbic acid and some of its derivatives had some deleterious effects on certain types of malignant tissues. It is also fair to say that intakes of vitamin C improve the quality of life of cancer patients. It becomes invaluable, however, after classical treatments like surgery, radiation and chemotherapy, pro-

vided the latter does not interfere with the ascorbic acid.

Some twenty years ago, the role of vitamins and the need of their supplemental intake were not well understood in Croatia even among nutritionists. This is the reason why Zvonimir Maksić and Mirjana Eckert–Maksić decided to translate Pauling's bestseller "How to Live Longer and Feel Better", Freeman & Co., New York, 1986. The book was a source of instructive and conclusive evidence about the need of using optimal amounts of vitamins in a healthy diet, if longevity and well–being is desired. The Croatian translation[64] appeared already in 1989 and was also a bestseller. It is important to point out that in the Afterword translators explicitly warn the readers that the general rules for determining optimal intake of vitamins do not exist and that they should be established on individual basis exercising a due care. The idea "more vitamins – better health" would be erroneous and potentially harmful. The book considerably contributed to a change in attitude towards vitamins in Croatia. It became optional literature at the Faculty of Medicine of the University of Zagreb. Both of translators got a lot of phone calls from people, who testified a beneficial influence of vitamins on their health and well–being, particularly in preventing common cold. Although this evidence was anecdotal, it has led to a feeling of inner pleasure and satisfaction, thus rewarding their efforts.

The Miraculous Proton

The proton is the smallest atomic nucleus and yet it plays a paramount role in acid–base chemistry, biochemistry and molecular biology. In Professor Maksić's words: "Little proton goes a very long way". He undertook massive *ab initio* calculations of the proton affinities some 15 years ago, which belong to the very first accurate calculations on large molecules.[65–69] In particular, polysubstituted aromatics were scrutinized and a simple additivity formula was found. It turned out that each substituent behaved as if others were not existent. The independent substituent approximation (ISA) is not only a rule of thumb, but has a predictive value,[70] *e.g.* in anticipating the place of the most probable electrophilic attack. The same rule *mutatis mutandis* works for deprotonation energies of the heavily substituted aromatics.[71,72] It follows as a corollary that the basicity and acidity of multisubstituted aromatics could be fully understood, if the effects of individual substituents would be grasped. This goal was accomplished much later by trichotomy formula, where protonation (basicity) and deprotonation (acidity) processes were broken down to three steps, which provided a sharp physical insight and greatly aided in interpretation of these two fundamental properties.[73,74] Trichotomy formula was applied to analysis of substituent effects, which were customarily correlated with empirical Hammett's σ–constants of various kinds. Triadic approach describes the influence of particular substituents by explicitly considering the ionization energies, relaxation energy and the association (or dissociation) bond energies to the proton,[75–77] which are common words in chemical laboratories. Combined with the additivity rules, it provides conceptually simple rationalization of basicity and acidity of highly substituted systems based on well defined physical entities. It is, therefore, not surprising that some researchers consider trichotomy analysis as the best available description of acid/base properties.[78]

The next step was computer design of strong organic superbases and superacids, which would have advantageous features compared to their inorganic counterparts and would act as powerful catalysts possibly in green chemistry. Following an in depth understanding of the protonation process, a simple strategy was developed for tailoring organic bases, superbases and hyperbases.[79–87] This strategy proved seminal and has led to a ladder of bases, which enters the realm of organic superacids (*vide infra*). Several proton sponges have been designed and synthesized[88–92] in collaboration with experimental chemists. The solvent effects on solvated superbases in acetonitrile have been well reproduced by the polarized continuum model.[93–95]

An analogous approach was found useful in tailoring organic superacids with a distinct difference that starting materials were already prepared known compounds, which served then as molecular backbones. Subsequently, the latter were dressed by suitable substituents except at the C–H or N–H bonds, which have been selected as excellent proton donors being placed at specific positions. It turned out that the most efficient acidifier was the cyano group due to its high electron acceptor power and modest steric requirements. It was conclusively shown that one of the most important factors determining the strength of superacids was accommodation of the excess negative charge in conjugate bases. The anionic resonance, triggered by deprotonation and supported by the cyano groups, exerts predominant effect irrespective of antiaromatic or aromatic character of the planar molecular skeleton. A large number of superacids was predicted[96–103] spanning the deprotonation energies in the gas–phase from threshold of superacidity (300 kcal mol^{-1}) to the threshold of superbasicity (245 kcal mol^{-1}). The latter value was suggested to be a gauge of hyperacidity at the same time.[104] By the same token, the threshold of superacidity is also recommended as a gauge of hyperbasicity.[104]

To epitomize, it was shown that basicity and acidity of organic compounds can be controlled in a remarkably simple way leading to the tailor–made superacids and superbases. Two important results have emerged from these studies of basicity and acidity: (1) a unified Jacob's ladder of all acids and bases was formed with superbases climbing up and superacids descending down on its rungs and (2) the excess charge in proto-

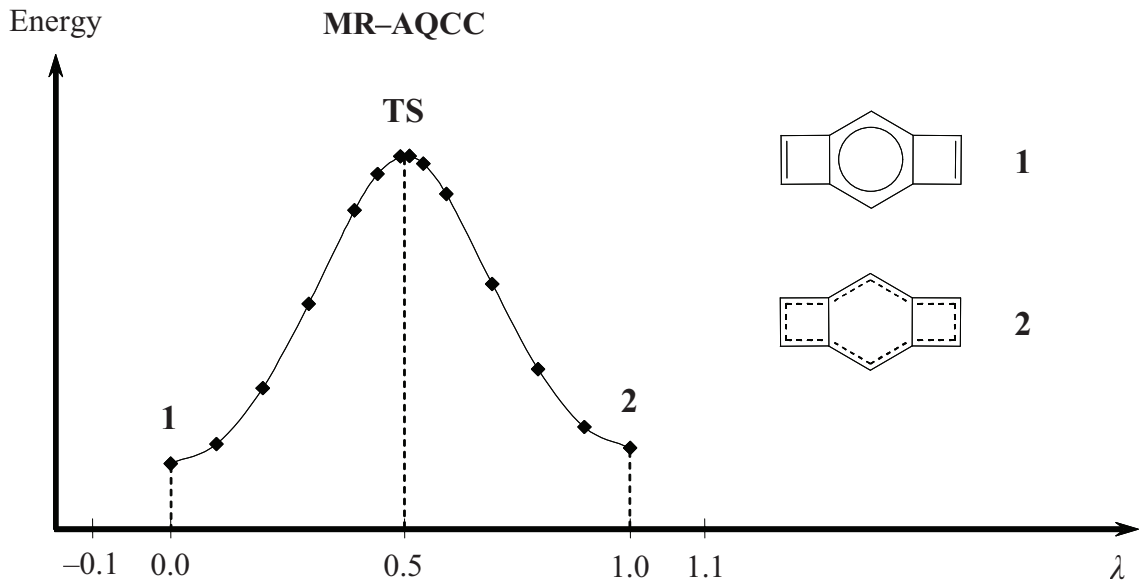

Figure 1. Schematic presentation of the barrier for the isomerization process between the bond–stretch isomers **1** and **2**. The total molecular energy changes are given against the generalized reaction coordinate determined by the parameter λ in a linear synchronous transit method (see reference 108). The transition structure is denoted by TS. Compounds **1** and **2** could be equally well termed as Bošković's isomers, since they are compatible with his idea about specific forces acting between atoms.

nated organic superbases and deprotonated superacids is so efficiently dispersed that they can form only weakly bound ion–pairs, which might be very useful in constructing new materials. This avenue of research is promising and should be exploited in the future.

The Benchmark Computations

Professor Maksić started with small desk calculator, but once the high performance supercomputers became available, he availed himself of new opportunities to enter a new field of the cutting edge computational chemistry. A large number of projects accepted by the John von Neumann Institute for Computing (NIC) in Jülich, Germany enabled use of one of the largest and the fastest supercomputers in Europe, which considerably increased the scientific productivity of the Quantum Organic Chemistry Group (QOCG) he founded at RBI. These projects put Zagreb on the map of the carefully selected users of the NIC supercomputing facility (at the moment with petaflop efficiency). Within this context, it should be mentioned that Professor Maksić was one of the speakers at the Second NIC Symposium in Jülich (17–18 February 2004), where highlights of the research activities of the Institute and the most important results have been presented.[105]

Highly accurate calculations *e.g.* carried out by the Multireference Average Quadratic Coupled Cluster (MR–AQCC) method are capable of revealing subtleties of the chemical bonding, which are not easily amenable to experimental examinations. One of those is a phenomenon called bond–stretch isomerism. Two bond-stretch isomers differ only in a distance of one or several bonds.[106] With a slight stretch of imagination this reminds to an old idea of Ruđer Bošković – a priest and a renowned mathematician, astronomer and physicist of the 18th century – who considered atoms as centres of force. The latter followed an oscillatory dependence against the interatomic distance.[107] The positive and negative values of the interatomic force meant repulsion and attraction, respectively. In between, the force assumed the zero values corresponding to the equilibria. In other words, two atoms were able to possess several equilibrium distances, which should explain different behaviour of atoms in the solid, liquid and gas phases. The atoms are supposed to oscillate around the equilibrium distances.[107] Obviously, Bošković's picture of the matter was a dynamical one. Going back from Bošković in the past to present days, it should be emphasized that some molecules do exhibit bond–stretch isomerism, implying that they differ just in the bond distances of several covalent bonds. A typical example is given by benzo[1,2:4,5]dicyclobutadiene **1** and **2** (Figure 1).[108] The isomer **1** has a pronounced aromatic character in the central benzene moiety and has two peripheral highly localized double bonds. On the other hand, isomer **2** has the π–electrons delocalized over the molecular perimeter representing the best realization of the 10 π–electrons in [10]–annulene.[108] The structural differences in **1** and **2** are found only in the C–C bond lengths, which holds throughout the isomerization reaction. The equilibrium structures **1** and **2** are therefore true bond–stretch isomers, which could be equally well

termed as Bošković' isomers. The forces acting at the nuclei are equal zero in the most stable geometries of **1** and **2**. Hence, they represent a polyatomic generalization of Bošković's two–atomic case! A specific example of the bond–stretching reaction is given by automerization of cyclobutadiene by π–bond flipping (shift) mechanism.[109] An interesting finding is that if the barrier height is not high enough, two bond–stretch isomers form a fluxional system like in the case of dicyanocyclobutadienes[110] in harmony with the early Bošković's dynamical picture.[107] Professor Maksić is trying to bring the problem of the bond–stretch isomerization into a focus of the chemical community. In a non–strict sense this rare and elusive phenomenon is related to Bošković's Law of Force, which is not precise in its details, but valuable in its conceptual content.

We have attempted to bring some characteristic issues into focus to illustrate several stages in his career, but this review would not be complete without Mills–Nixon controversy. It mirrors his fearless fight for scientific truth at all costs against many opponents including some Editors. The Mills–Nixon effect (MN) story started some eighty years ago[111] by noticing that small strained rings annelated to the benzene fragment cause a typical orientational effect in directing the preferential electrophilic attack. This hypothesis was vindicated by carefully designed calculations on model molecules and real compounds[112–115] yielding results in agreement with experimental findings. The structural changes induced by fusion of small rings[116–119] were correctly reproduced and interpreted in terms of the rehybridization at the carbon junction atoms and additional (hyper)conjugation effect(s). Despite quite convincing evidence there were quite some researchers, who produced counter "arguments" claiming that the MN effect was not existent. Subsequently, they had to admit that the effect was real, but "so small that it was not relevant". This allegation was not correct. On top of this, to make bad situation worse, one author "reinvented" Mills–Nixon effect and termed it differently, which was ethically unacceptable. We shall not mention the names, but they can be found in an eloquent, clear–cut and scholar review article.[120] Moreover, by using modelling as a guiding principle, Zvonimir Maksić and co–workers found systems, which exhibited reversed Mills–Nixon effect.[121–126] Some of these systems were prepared in laboratories by Japanese synthetic chemists.[127–130] Their structural characteristics and reactivity in the electrophilic substitution reactions are diametrically opposite to that found in the MN–systems. The arguments, vigour, persistence and the truth itself prevailed at the end and have led to some new knowledge.

The Editorial Work

Professor Maksić never missed opportunity to stress importance of models, concepts and interpretation of the results produced by theory, computations and experiments. In his words models and concepts are chemists' best friends. They are "forever like diamonds". The role of Linus Pauling, John C. Slater and Charles A. Coulson in their development was crucial. In order to keep balance between computational and conceptual quantum chemistry Professor Maksić has edited two special issues of *Croatica Chemica Acta* (CCA) on the conceptual approach in chemistry a quarter of century ago.[131] These two volumes were close to the leading edge of interpretational side of quantum chemistry. He was able to attract as contributors many grandmasters and masters of modelling in chemistry: Linus Pauling and his main theoretician at The Linus Pauling Institute of Sciences and Medicine in Palo Alto – Zelek S. Herman, followed by Carl J. Ballhausen, Lawrence S. Bartell, Mikhail V. Basilevski, Krishnan Balasubramanian, Fernando Bernardi, Jeremy K. Burdett, Dieter Cremer, Boris Galabov, Dušan Hadži, Edgar Heilbronner, Ivan Hubač, Gilles Klopman, Elfi Kraka, William L. Luken, Leo Klasinc, John N. Murrell, Roy McWeeny, Hiroshi Nakatsuji, Eiji Ōsawa, Gabor Náray–Szabó, William E. Palke, Peter R. Surjan, Jacopo Tomasi and Nenad Trinajstić. It is a great pleasure indeed that some of them are also authors in the present Festschrift. After an intermezzo with the book on the Modelling of Structure and Properties of Molecules,[132] his editorial work on the modelling of the chemical bond was crowned by a series of books *Theoretical Models of Chemical Bonding*.[133] It is a four–books story of the chemical bond, which is so versatile and omnipresent, that it provides the very basis for chemistry, molecular crystals and materials as well as a foundation for the living matter. Its modelling is a search for simplicity, insight and understanding, which offers Ariadne's thread through the labyrinth of myriads of data.[134] This series found its place on the shelves of many libraries all over the world. The Editor–in–Chief of the famous *Encyclopedia of Quantum Chemistry* Paul Schleyer wrote in the Introduction that the series *Theoretical Models of Chemical Bonding* is a useful supplementary literature to the *Encyclopedia*.[135] Postgraduate and postdoctoral students of chemistry are well advised to study this series, since it has a lasting value.

The last three decades have witnessed a slow but permanent scientific revolution which is called computational sciences. It is a result of the advances in computer technology and progress in solving quantum many–body problems. As a result it can be safely concluded that the computational sciences: (1) united a great deal of physics with chemistry and molecular biology and (2) provided the third pillar of natural sciences in addition to the already existing experiment and theory. The computational science yields results often of

equal or better accuracy than experiments. It is applicable in situations, which cannot be realized in laboratories, thus giving valuable supplementary information. It is gratifying that the computational quantum chemistry is one of the most important avenues of the computational sciences. In order to contribute to this historical development Zvonimir Maksić and Peter Politzer started a new series of books in 1994, called *Theoretical and Computational Chemistry*.[136] It reflects much of advances in theoretical chemistry and its computational applications in the last decade of the last and the first decade of the 21st century. It is impossible to describe here the whole series and its many highly valuable books. If we have to single out just one topic, then we would mention two volumes of Peter Schwerdtfeger's *Relativistic Electronic Structure Theory and Applications*,[137,138] because it is the first *in depth* and *in extenso* treatise on the relativistic effects in molecules.

This is not all! Professor Maksić edited several special issues or books honouring eminent scientists like Linus Pauling,[139–141] Per O. Löwdin,[142] Clemens C. J. Roothaan and George G. Hall,[143] and Dušan Hadži.[144–146] Several special issues are dedicated to important symposia.[145–149] Particularly interesting documents on the historical events in the South–East Europe at the end of the last century are volumes of the *Journal of Molecular Structure*[145,146] representing papers of the 20th European Congress on Molecular Spectroscopy, which should have been held in Zagreb, Croatia, 25–30 August 1991, but was cancelled in the last minute, because of the "balvan (balk) revolution" and subsequent aggression on Croatia after declaration of its independence. The scientific messages of the Congress, which did not take place, are preserved in these volumes.

Finally, the 120th anniversary of Van't Hoff's tetrahedral carbon atom was celebrated in a special issue of the *Journal of Molecular Structure THEOCHEM*.[150]

Teaching and Visiting Professorships

His teaching career starts with Božo Težak,[151] professor of physical chemistry at the Faculty of Science in Zagreb, a man of a broad culture, wide horizons, foresighted visions, integrity and courage. He was much ahead of his time with his bold views. This journal changed its name to *Croatica Chemica Acta* thanks to his Gargantuan's efforts. It was not easy to do it in the former communist Yugoslavia. As the Editor–in–Chief, he changed the language to English and introduced a documentation card, which facilitated transmission of the information to the Chemical Abstracts. The CCA was the first scientific journal in the world possessing documentation cards, which was important innovation at that time. Božo Težak also tried to modernize the physical chemistry curriculum at University of Zagreb and offered part time positions of associate professors to four young scientists of the Ruđer Bošković Institute: Tomislav Cvitaš, Leo Klasinc, Zvonimir Maksić and Nenad Trinajstić in 1973. The offer was gladly accepted, which has led to considerable improvement in teaching of molecular spectroscopy, mathematical methods in chemistry, quantum chemistry and chemical documentation. Professor Maksić has been teaching many undergraduate courses in his long term academic career, as well as two postgraduate courses: advanced quantum chemistry for chemists and quantum theory of atoms and molecules for physicists. The common denominator of his lectures was enthusiasm and a flavour of research, since he frequently discussed the most recent developments in quantum chemistry including some of his own results. In this way he gained a number of good students willing to do their diploma theses under his guidance. The results of these works were published in good journals as a rule. His hallmarks were sentences like "Listen to your teachers very carefully, but always make up your own mind" or "Never be afraid or ashamed to admit that you do not know or understand something. This is the first step of learning." He published two students–friendly textbooks based on his lecture notes: *Kvantna kemija* (*Quantum Chemistry*), Liber, Zagreb, **1976** and *Simetrija molekula* (*Symmetry of Molecules*), Školska knjiga, Zagreb, **1979** (together with L. Klasinc and N. Trinajstić). For his teaching he received a Medal of the Department of Chemistry, Faculty of Science in 2005.

Zvonimir Maksić visited many universities and institutes particularly in Europe. He went on lecturing tours and gave lectures at universities in Europe as South as Rome and Barcelona, and as North as Trømse in Norway within the polar circle. The pinnacle was, however, the 22nd Annual Charles A. Coulson lecture at the Department of Chemistry in Athens (Georgia, U.S.A.) in September 2008, named after one of the founders of the conceptual quantum chemistry. This lecture is considered as a great honour, since it was held by many prominent scientists in the past including Nobel laureates John A. Pople and Ahmed Zewail. Athens is known as a home town of the world's leading Center for Computational Quantum Chemistry, where the computational science is exercised at its finest, led by Henry F. Schaefer III, Paul von Ragué Schleyer, Norman L. Allinger and Wesley D. Allen. Professor Maksić received a plaque for his "pioneering contributions to the understanding of the chemical bond" (Figure 2).

He was guest scientist at several universities abroad like Münster, Germany (Martin Klessinger) and Madrid Cantoblanco, Spain (Manuel Yáñez and Otilia Mó), but the often repeated longer stays at the University of Heidelberg were exceptional and rewarding experience, which had a profound influence on his re-

Figure 2. Plaque presented to Zvonimir Maksić after his Charles A. Coulson lecture in September 2008.

search. He found a long lasting interaction with Professor Rolf Gleiter highly stimulating and his friendly advice, criticism and encouragements were extremely helpful.

Service to the Scientific Community

Zvonimir Maksić never refused to be a servant of science. He was a member of the Board of Governors at RBI in two terms (1994–1995 and 2004–2006), head of the Department of Chemistry at RBI (1995–1997), deputy director general of RBI (1997–1999). He was one of the founding fathers of the Croatian Humboldt Club and its vice–president (2004–2006). He is the incumbent president of the Collegium Emeritorum at RBI, former member of the Editorial or Advisory Boards of *Journal of Molecular Structure THEOCHEM*, *Structural Chemistry*, *International Journal of Quantum Chemistry*, *Croatica Chemica Acta* and *Encyclopedia Moderna*. As to *Croatica Chemica Acta*, he was a member of the Board for some 20 years (1976–1994). It was his idea that CCA should introduce special topic issues, which was at the end accepted thanks to a strong support of the Editor–in–Chief dr. Siniša Maričić. He was the president of the Croatian Chemical Society (CCS) 1988–1990. Professor Maksić tried to strengthen ties with other Chemical Societies, and after his proposal "Božo Težak" medal was introduced as the highest recognition for scientific achievements in chemistry of the Croatian Chemical Society. The first recipients of the medal were Nobel laureates Linus Pauling (1988) and Vladimir Prelog (1989). Further, he was a member of the IUPAC Commission on Molecular Structure and Spectroscopy and a member of the Management Committees of the COST actions D9, D26 and D37. He is currently a member of the Management Committee of the Division of Computational Chemistry of the European Association for Chemical and Molecular Sciences (EuCheMS). Last but not least, he was promoter of the Ph.D. Honoris Causa procedure for Linus Pauling at the University of Zagreb in 1988.

Finally, it is noteworthy that he organized or was a member of the Organizing Committee of several symposia.[152–157] In particular, it should be mentioned that he is one of the founding fathers and member of the Standing Committee of the Central European Series of Conferences "Chemistry towards Biology".

Disarmament and Peace Initiatives

Zvonimir Maksić is a member of the Croatian Pugwash Movement founded by Ivan Supek. He is follower of Linus Pauling's point of view that scientists with their knowledge should serve society and have particular

responsibility to the tax–payers. In 1988 a very important symposium on the electronic structure of molecules, clusters and crystals was organized by Professor Maksić in Cavtat (Croatia), including pleiad of theoretical chemists. The main plenary lecture was given by Linus Pauling followed by a talk of Ivan Supek on Ruđer Bošković and his anticipation of modern science.[158] Both Pauling and Supek were pronounced members of the international Pugwash Movement. In addition to scientific issues, global problems faced by the World were discussed too, as described by Professor Maksić in his reminiscences two decades after.[159] He was entrusted to organize the first meeting and to prepare the first draft for the topics to be considered for an *ad hoc* Committee including L. Pauling (president), I. Supek (vice–president), K. Fukui, P. O. Löwdin (member of the Nobel prize Committee), R. McWeeny, P. Fulde, C. C. J. Roothaan, J. Roothaan and Z. Maksić. The first version of the Cavtat Declaration was put together and presented to the participants at a special plenary session. The final text including suggestions made during general discussion was signed by participants with very few exceptions. The Cavtat Declaration (http://spider.irb.hr/CCA_ZBM/Cavtat_declaration.pdf) was born and published in *Croatica Chemica Acta* **1989**, *62*, III–IV; *International Journal of Quantum Chemistry* **1989**, *36*, 1–3; *Vjesnik of the Croatian Academy of Sciences and Arts* **1992**, *32*, Nos. 7–8; and *Priroda* **1988/89**, *No. 2*, 2. It was discussed by some participants in public and in the media in Croatia and many countries abroad. It was particularly well accepted by Polish scientists fighting for political freedom in Poland. The declaration is an appeal for an action for human survival and preservation of the life on Earth. It is a warning against four apocalyptic dangers: the armament race, the economic collapse at the global scale, ecological catastrophe and the overpopulation bomb. It is a strong plea for a complete disarmament with an emphasis on the nuclear weapons. The saved money could and should be used in social programs, better health care, support of education and science. The Cavtat Declaration is as timely as ever, since the crisis the world is going through nowadays was predicted two decades ago. It was a strong voice raised for international collaboration in saving this planet and sign–post for younger generations. It is encouraging that the president of the United States Barack Obama started to talk about the world without nuclear bombs and about "green Earth" with ecological energy sources. Twenty most powerful economical countries (G20) initiated measures to curb the world crisis. Neither of that is a direct consequence of the Cavtat declaration. Nevertheless, the latter convincingly shows that scientists should take an active part in shaping the future of the world. This is their moral obligation.

The fall of the Berlin wall occurred just a couple of years after the Cavtat Declaration. It was followed by the collapse of Yugoslavia and Soviet Union. The economic and political tensions between the republics in Yugoslavia and demand for political freedom and democracy were too strong to keep the artificial state alive. The republics used the constitutional right to declare independence, but Belgrade reacted by invasion of Slovenia, Croatia and Bosnia–Herzegovina by the pro–Serbian so called Yugoslav Peoples Army (JNA). Particularly brutal war has taken place in Croatia and Bosnia–Herzegovina due to Serbian paramilitary units. Zvonimir Maksić asked Linus Pauling to do something about it, because he was not only one of the leading scientists, but also a great moral authority in the world as a Nobel prize winner for peace in 1962. Professor Maksić was constantly in touch with his friend and Pauling's coworker Dr. Zelek Herman. Finally, Dr. Herman sent him an Appeal for Peace in Croatia signed by Linus Pauling. It was written, as it later turned out, by Ivo Banac, professor of history at Yale at that time.[160] Pauling's signature was a trigger for a wide action of Nobelists for Peace in Croatia.[161] This action was coordinated by Dr. Greta Pifat–Mrzljak (RBI), whose role was impossible to overestimate.[161] Particularly instrumental was very active participation of the nobelists Robert Huber and Manfred Eigen, who were engaged by Dr. Pifat–Mrzljak. The appeal was a great success, since it was signed by more than 120 Nobel Prize winners. It has helped to calm down the unscrupulous Serbian propaganda in the world. A large number of scientists at RBI and Croatian Diaspora took part in peace efforts by writing letters to the leading politicians explaining the nature of the conflict in the former Yugoslavia.[162]

The situation in Bosnia–Herzegovina went from bad to worse in 1992. A new independent country was exposed to aggression by the pro–Serbian JNA and Serbian paramilitary troops threatening to escalate to genocide of cataclysmic proportions. More than 1 million of refugees and displaced persons poured to Croatia, which was under attack itself being endangered too. The pattern of destruction and ethnic "purification", later called "cleaning" by some politicians, revealed plans for formation of the Greater Serbia. Zvonimir Maksić wrote a strong text entitled "An Appeal for Peace in Bosnia and Herzegovina and Stability in the Balkans" in may 1992 (http://spider.irb.hr/CCA_ZBM/Appeal_BaH.pdf). It is pointed out that Belgrade is an epicentre of permanent instability in the Balkans and that all necessary measures should be undertaken for its pacification. Human solidarity demands an immediate action against the aggressor in order to save human lives and to alleviate misery and suffering. The borders of democratic coun-

tries should be kept open for agonizing refugees. The democratic processes should be strongly encouraged and supported in the Balkans as a factor of peace and stability. It is noteworthy that onslaughts like that in Srebrenica and later events in Kosovo were predicted already in May 1992. Zvonimir Maksić approached Abdus Salam (Nobel prize in physics in 1979), the director of the Theoretical Physics Institute in Trieste, and got his full support and the first signature. Next signatories were Vladimir Prelog (born in Sarajevo!), Linus Pauling and many others making 84 Nobel laureate supporters in total. Appeal was sent to many leading politicians. Their answers were very supportive. We shall illustrate it by a letter of the Secretary General of the Council of Europe in Strasburg Mrs. Catherine Lalumière (http://spider.irb.hr/CCA_ZBM/Letter_Lalumiere.pdf). Mrs. Lalumière pointed out that she shared completely concerns expressed in the Appeal. It was emphasized that the Council will work with Governments to put an end to hostilities and to the construction of civilized world when arms have been silenced. The accompanying documents were related to formation of "safe heavens" and measures necessary to be undertaken in helping refugees. Unfortunately, politics and diplomacy were too slow to save people in the "safe heaven" of Srebrenica. Both Appeals for peace in Croatia and Bosnia–Herzegovina addressed one of the greatest moral issues in Europe in the last decade of the 20th century trying to stop aggression and ensure human rights of minorities and deprived people. They reflect the responsibility, which scientists have in building a safer world and better future for the mankind as strongly emphasized in Cavtat declaration.

Instead of an Epilogue

Zvonimir Maksić is a prolific scientific author. He published some 250 papers and 23 review articles and chapters in monographs, which have been cited in primary and secondary publications for more than 3.500 times. Importantly, 96 of his papers were published in journals with very high impact factors. For his work he received several prizes and honours. We shall mention only City of Zagreb award for science in 1976, National award of Croatia for excellence in natural sciences in 1987 and National award of Croatia for the life achievements in natural sciences in 2009. He became distinguished scientist at RBI in 2005 working with youthful zest being as productive as ever, implying that his scientific journey is still going on. The exhibited curiosity is astonishing and new ideas are never ending. His enthusiasm is catching and stimulating. One can expect a lot of interesting results on amino acids, small peptides and nucleic acid bases both in the gas–phase and water solutions. Some surprises cannot be excluded. We can also look forward to new simple and elegant interpretations of molecular phenomena, which are still not well understood. Have a long and nice journey Professor Maksić!

Davor Margetić

Robert Vianello

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