



CROATICA CHEMICA ACTA
 CCACAA, ISSN 0011-1643, e-ISSN 1334-417X
Croat. Chem. Acta **82** (4) (2009) 791–800.
 CCA-3373

Author's review

Positronium – Hydrogen Like and Unlike*

Milan Randić**

National Institute of Chemistry, Ljubljana, Slovenia
 (E-mail: mrandic@msn.com)

RECEIVED SEPTEMBER 2, 2008; REVISED JANUARY 13, 2009; ACCEPTED MARCH 30, 2009

On the occasion of the 2008 Brijuni Conference on Hydrogen – the most abundant atomic species in the Universe, it seems fitting to draw attention of the participants of this conference, as well as chemists at large, to Positronium – one of the least abundant atom-like species in the Universe, if for no other reasons then because it was theoretically predicted by a Croatian scientist, Stjepan Mohorovičić some 75 years ago, about 100 miles away, in the city of Zagreb, the capitol of the Republic of Croatia.

Abstract. A brief review on positronium, Ps, hydrogen-like system built from positron and electron, is outlined from its beginning in 1935, the first theoretical study on this relatively stable matter-antimatter system by Stjepan Mohorovičić, to the most recent works on positronium hydride PsH, and positronium molecule Ps₂, analogue of hydrogen molecule. Mohorovičić calculated spectra of Ps and was even looking for it in the sky searching for its spectrum, but experimental observations of positronium Lyman- α radiation Ly α λ 2430 line waited for another 40 years before being successfully identified in a laboratory in 1975 by Canter and collaborators. It took another ten years for astronomical observation of the presence of positronium in outer space in 1984 by McClintock, who observed Ly α λ 2430 line in spectra of Crab Nebula, 50 years after the attempts of S. Mohorovičić to detect positronium lines. The work of Mohorovičić was mostly ignored in his native Croatia, until the most recent time, an illustration of “historical blunder” of local physics community – phenomenon not so unheard of in science in general, as has been recently worldwide illustrated with hesitation of acceptance of the notion of nonlinear dose response (hormesis); the density functional theory; and chemical graph theory.

Keywords: positronium, positronium hydride, molecular positronium

INTRODUCTION

“The father of positronium,” Stjepan Mohorovičić, was born in 1890 in Bakar, a small coastal city of Croatia some 63 miles (100 km) from Brijuni and died at the age of 90 in Zagreb. At best he had a miserable acceptance by local scientific and local political authorities, and was prevented by different and opposing political regimes admittance to be a faculty at Zagreb University, despite the prestigious position of his father at the University. Stjepan Mohorovičić is son of the famous Croatian geophysicist, Andrija Mohorovičić (1857–1936), born in Volosko, another small coastal town of Croatia, less than 30 miles from Brijuni, who predicted the MOHO layer (a discontinuity at the boundary between the Earth crust and the mantle). Andrija Mohorovičić was

also first to measure fluctuations between tide and ebb of the Adriatic Sea, and initiated measuring of variations in ozone in the atmosphere in Zagreb, about 80 years ago, when few even heard of the problems of ozone.

Recognitions of accomplishments of a scientist by their contemporary colleagues are uncommon even when the work is in commonly recognized areas of science, and scientists are in the leading institutions and the leading scientific countries of the world. But for a scientist from an “unheard” of country, and an “unheard” of university, or no university at all, as has been the case with Stjepan Mohorovičić, the “father of positronium,” a proper recognition of their scientific accomplishment is beyond reality. On the top of this, Stjepan

* This contribution is dedicated to the memory of my physics teachers, Marija Lukšić (high school teacher), Mladen Paić (1905-1997), Branimir Marković (1917-1973), Vatroslav Lopašić (1911-2003), Milena Varičak (1903-1971), Ivan Supek (1915-2008), Zlatko Janković (1916-1987), Ivan Babić-Gjalski (1925-1953), Vladimir Glaser (1924-1984), Borivoj Jakšić (1925), Krunoslav Ljolje (1928-1994) and Aleksandar Grossman (1930) at the University of Zagreb.

** Visitor; Permanent address: Emeritus, Department of Mathematics and Computer Science, Drake University, Des Moines, IA 50311, USA.

Mohorovičić has additional burden to face, living in the shadow of his father, a famous and recognized scientist. However, there is no doubt that Stjepan Mohorovičić was outstanding scientist and that his work was one of the most outstanding accomplishments of Theoretical Physics of the early Quantum Theory period. How little was known of his work, although it has been published in respectable scientific journal, is seen from the fact that on two occasions his calculations were re-produced. The title of the paper of S. Mohorovičić:¹ “Möglichkeit neuer Elemente und ihre Bedeautung in Astrophysik” (Possibility of novel elements and their meaning in astrophysics) is indicative that S. Mohorovičić was fully aware of the significance of his work. For an introduction to the discovery of positronium see a brief review² by Helge Kragh entitled: “From “electrum” to positronium.” In addition there are two similar “popular” articles in Croatian language by H. Galic³ and V. Paar⁴ about Stjepan Mohorovičić and positronium. I may add that during the four years of being student of Theoretical Physics at the University of Zagreb, the name and the work of Stjepan Mohorovičić was never mentioned, even though his work has been known to few abroad. An exception in Croatia was Professor Vladimir Glaser, who in his book on quantum electrodynamics, published in 1955 in Croatian language,⁵ has mentioned the work of Stjepan Mohorovičić on positronium. In passing, the book of V. Glaser was one of the first monographs on quantum electrodynamics ever published. It was published three years before the book edited by J. Schwinger “Selected Papers on Quantum Electrodynamics”,⁶ and 30 years ahead of the “classic” of R. P. Feynman: “Quantum Electrodynamics: The Strange Theory of Light and Matter”.⁷

At this point it is worthwhile to recall a comment of Vannevar Bush (1890–1974), an engineer who developed the differential analyzer (analog computing) in 1928 at MIT, and was influential government advisor and science administrator. He referred to Mendel in the following way:

“...Mendel's concept of the law of genetics was lost to the world for a generation because his publication did not reach the few who were capable of grasping and extending it; and this sort of catastrophe is undoubtedly being repeated all around us, as truly significant attainments become lost in the mass of inconsequential.”

The case of Stjepan Mohorovičić is different in the sense that his work did *reach the few who were capable of grasping and extending it* but the importance of his significant attainment became almost lost for his immediate contemporaries in Croatia and the innocent generation that followed, even though eventually his major accomplishment, the postulate on existence of positronium, being known abroad, could not but be “redisco-

vered” at home, sooner or later. From my correspondence with Academician Paar I learned that it was sooner thanks to an “accidental” contact between Academician V. Paar (theoretical physicist) and Professor Krešimir Balenović, the head of organic chemistry at the University of Zagreb. Professor Balenović draw attention of V. Paar to Stjepan Mohorovičić, who had been teaching physics in a high school attended by Balenović many years back. Professor Balenović was somewhat irritated by complete disregard among contemporary Croatian physicists for his former physics teacher, Stjepan Mohorovičić, as if he did not exist. This disregard went so far that around 1950 none of the physicists of the University of Zagreb with a scientific reputation was willing to testify that Stjepan Mohorovičić is *bona fide* scientist (who had about dozen publications in reputed German astrophysics journals). This “don't see, don't hear, don't speak” attitude towards Mohorovičić deprived Mohorovičić to qualify for a better retirement pension, to which scientist have right to apply. Today's interpretation of the three wise monkeys: “See no evil, hear no evil, speak no evil,” according to Wikipedia, is commonly used to describe persons who do not want to be involved in a situation, persons turning blind eye to the immorality of an act in which they are involved – and for reasons that remain unknown that appears to be the position of then the scientific (physics) “Establishment” in Croatia. It also appears that Vladimir Glaser, who has been the best among theoretical physics in Croatia at that time and the time that followed, was the only person who knew better.

The paper on Positronium of Stjepan Mohorovičić,¹ particularly when viewed from the present time, could have been worthy of the Nobel Prize. At first sight this may appear as an exaggeration if not a preposterous speculation, but enough time has passed that in retrospect one can better appreciate the importance of the “discovery” than would have been possible 70 years ago. As we know today the postulate on positronium has lead to novel insights in physics, goes beyond positronium not only as a component in search for elusive antiproton, detected in cosmic rays about 30 years ago,⁸ which is the core of antihydrogen, a counterpart of hydrogen,^{9–11} for arrival at “hybrid” molecules, parts consisting of atoms and parts of positronium (Ps), like positronium hydride PsH,¹² lithium positronium PsLi,¹³ and of recently opened the field of molecular positroniums Ps₂.¹⁴ One can view this in parallel with the discovery of buckminsterfullerene, C₆₀, by Curl, Kroto and Smalley in 1985,¹⁵ for which they shared Nobel Prize in 1996. Few have thought in the mid 1980s that this novel allotrope of carbon, despite that it revolutionized our knowledge on carbon, would be more than a interesting curiosity of chemistry, such as is, for instance bullvalene, C₁₀H₁₀ molecule, conceived by von Doering and Roth¹⁶

and synthesized the next year by Schroeder,¹⁷ a molecule in which at room temperature “all ten carbon atoms inevitably wonder over the surface of a sphere in ever changing relationship to each other”.¹⁶ Formally, bullvalene molecule has $10!/3$ or 1,209,600 valence structures and at the room temperature fluctuates between these structures, the interconversions between which lead to a cubic degenerate rearrangement graph having over one million vertices and which has been referred to as the “monster” graph.^{18–22} Buckminsterfullerene and bullvalene demonstrate that first impressions may be misleading, that what may appear as a curious, peculiar, unusual, exotic, unconventional and exceptional may grow into promising and prominent, impressive and important, noteworthy and extraordinary novelty. As we witness today the chemistry of fullerenes and the chemistry of bullvalenes have developed and both fields have expanded considerably, so much so, that this is visibly even to laymen. Positronium appears that it might follow the same fate.

The fact that Stjepan Mohorovičić has not received the Nobel Prize has deprived Croatia for the third time of the Nobel Prize in Physics. Stjepan Mohorovičić shares the fates of the geniuses of Nikola Tesla (1856–1943), and his father Andrija Mohorovičić (1857–1922). Nikola Tesla and Andrija Mohorovičić are today fully recognized by all, but at the time of living apparently they have not been recognized for their outstanding accomplishments. Moreover, in the case of Tesla, the “injustice” has been augmented by the fact that Guglielmo Marconi, who shared Nobel Prize in physics in 1909 with Carl Ferdinand Braun, “*in recognition of their contribution to the development of wireless telegraphy*” has built in his radio 17 of Tesla patents. Perhaps the only satisfaction that Tesla could have had was that finally over thirty years later, in 1943, the U. S. Supreme Court upheld Tesla’s radio patent over that of Marconi, but unfortunately this decision came months after Tesla died.

The case of Tesla is not the only instance that high courts have resolved the issues of priority in science. The Circuit Court in Chicago has resolved the issue of the invention of the first electronic computer, which was not ENIAC (Electronic Numerical Integrator And Computer), World’s first general-purpose electronic computer, built by John Mauchly and John Eckert at the University of Pennsylvania in 1946, but the ABC (Attanasoff-Berry-Computer), built in 1939 at Iowa State University, Ames, Iowa. It was built for solving simultaneous linear equations, used electronic tubes and magnetic memory and manipulated binary numbers instead of decimal. The Circuit Court in Chicago has decided that the first computer was not invention of J. Mauchly and J. Eckert of University of Pennsylvania but of “some At-

tanassoff” from Iowa State University by the evidence that has shown that J. Eckert has spent a week in Ames Iowa in the laboratory of J. Attanasoff prior to construction of ENIAC. The case of Nikola Tesla and the case of John Attanasoff illustrate undesirable scientific blunders, individual blunders, affecting individual scientists. The same is the case with Stjepan Mohorovičić, except that his case illustrates *local* scientific blunders, which are even more difficult to understand because those in doubt and willing to clarify the situation could have contacted outside sources. Apparently during the long life of Stjepan Mohorovičić there were no such in Zagreb.

Speaking of scientific blunders, more troublesome are cases of “historical blunders,” cases in which *groups* of scientists, *not individuals*, devoted to various “controversial” topics are ostracized, ignored, rejected, excluded and prevented to participate as equal members of scientific community. They are treated by the scientific Establishment and their cohorts as pursuing pseudoscience and not *bona fide* science. Such incorrect, unethical, contemptuous, unscrupulous and arrogant attitude of self-appointed “influential” scientists tends unfortunately to be perpetuated by lack of involvements of majority of scientists, the inertia of the majority of scientists to get involved in things of which they may be uninformed or misinformed, unfamiliar, unacquainted, inexperienced, uninterested, unenthusiastic, or unresponsive as being beyond their limited research interests, all which favors *status quo*. However, eventually these “houses of cards,” maintained by Establishment will collapse, just as are bound to collapse speculative schemes that depend on unstable factors that the planner cannot control. In this respect we may recall a statement of Sigmund Freud (1856–1939):

“The voice of intellect is a soft one, but it does not rest until it has gained a hearing. Ultimately, after endless rebuffs, it succeeds. This is one of the few points in which one may be optimistic about the future of mankind.”

HISTORICAL BLUNDERS

One should not insinuate unfairness and blame the Swedish Academy of Sciences for not awarding the Nobel Prize to these giants of the Croatian Science. The blame and the shame is on the contemporary physicists, who were blind “to see the light” when the light was shining and to make nominations and adequate recommendations to the Swedish Academy of Sciences. The euphemism “not to see the light” can be better characterized in a plain language as blunder. In view of the historical significance of positronium here we can speak of

Table 1. Nobel Prize in physics for discovery of new particles and their properties

Scientists	Nobel Prize	Physics
Lord Raleigh	1904	Discovery of argon
A. Einstein	1921	Laws of photo effect
W. Heisenberg	1932	Interalia for discovery of allotropic forms of hydrogen
Sir James Chadwick	1935	Discovery of positron
O. Stern	1943	Discovery of magnetic moment of protons
I. I. Rabi	1944	Magnetic moments of atomic nuclei
C. F. Powell	1950	Discovery of mesons
P. Kusch	1955	Determination of magnetic moment of electron
E. G. Segre O. Chamberlain	1959	Discovery of antiproton
B. Richter S. C. C. Ting	1976	Discovery of a heavy elementary particles of new kind
L. M. Lederman M. Schwartz J. Steinberg	1988	Discovery of muon neutrino
M. L. Perl F. Reines	1995	Discovery of tau lepton Detection of neutrino

Table 2. Nobel Prize in physics for discovery of new elements and their properties

Scientists	Nobel Prize	Physics
H. Moissan	1906	Isolation of flourine
M. Curie	1911	Discovery of radium and polonium
F. Soddy	1921	Origin and nature of isomers
H. C. Urey	1934	Discovery of heavy hydrogen
O. Hahn	1944	Fission of heavy nuclei
E. M. McMillan G. T. Seaborg	1951	Discovery of chemistry of transuranium elements
G. Olah	1994	Carbocation chemistry
F. Curl H. Kroto R. E. Smalley	1996	Fullerenes

historical blunder. Before elaborating on “historical blunders” in science let just buttress the statement that “the paper on Positronium of Stjepan Mohorovičić,¹ particularly when viewed from the present time, could have been worthy of the Nobel Prize,” by listing in Table 1 and Table 2 a selection of the Nobel Prizes in physics and chemistry, respectively, for discoveries that are of a similar kind, relating to “new matter,” though of

course each discovery has its own unique justification. Despite the “historical blunder” of their contemporaries, in not recognizing and not acknowledging Andrija and Stjepan Mohorovičić, for their monumental scientific accomplishments, Croatia nevertheless belongs to an exclusive club of countries, which includes the United States, France, United Kingdom, Denmark, Sweden and Germany, which have combinations father (mother) and

Table 3. Outstanding father-son, father-daughter and mother-daughter “family” scientists

Scientists	Nobel Prize	Discipline	Country
William Bragg	1915	Physics	United Kingdom
Lawrence Bragg	1915	Physics	
Niels Bohr	1922	Physics	Denmark
Aage N. Bohr	1975	Physics	
Arthur Kornberg	1959	Physiology-Medicine	United States
Roger D. Kornberg	2006	Chemistry	
Manne Siegbahn	1924	Physics	Sweden
Kai M. Siegbahn	1981	Physics	
Hans von Euler-Chelpin	1929	Chemistry	Sweden
Ulf von Euler	1970	Medicine	
J. J. Thompson	1906	Physics	United Kingdom
George Paget Thompson	1937	Physics	
Pierre Curie	1903	Chemistry	France
Irène Joliot-Curie	1935	Chemistry	
Marie Curie	1903; 1911	Physics; Chemistry	France
Irène Joliot-Curie	1935	Chemistry	
Andrija Mohorovičić		Physics	Croatia
Stjepan Mohorovičić		Physics	

son (daughter) as outstanding scientists (see Table 3).

“Historical Blunders” in sciences are not only the events of the past, as one would have hoped, but also of the contemporary age. The Hormesis, which claims the presence of a non-linear drug dose-response relationship for organisms (animals and plants) has been known for decades, yet the J-shaped dose-response relationship has been shunned for years by Pharmacology Establishment until a very recent awaking.^{23,24} Incidentally, not long ago a novel mathematical characterization and analysis of proteomics maps, initiated by this author,^{25–37} which can be viewed as a generalization of graph theoretical approaches developed for molecules, demonstrated for the first time the presence of the hormesis even at the proteome level (that is at the cellular level).³⁸

Another blunder of the near past concerns Quantum Chemistry, the self-appointed “Queen” of Theoretical Chemistry. The Density Functional Theory,^{39,40} the DFT, was undeservingly disregarded by an influential group of quantum chemistry “Establishment” till ten years ago.^{41,42} However, in 1998 Walter Kohn, one of the initiators of the DFT, shared the Nobel Prize in chemistry with John Pople, the proponent of the traditional quantum chemistry. Clearly, the Nobel Prize of Kohn could not be ignored, which brought the happy end to the ill fate of DFT! But Chemical Graph Theory, which had support and understanding of giants of Theo-

retical Chemistry, Charles A. Coulson (1910–1974), E. Bright Wilson (1908–1992), Per Olov Löwdin (1916–2000), Vladimir Prelog (1908–1998), and others, has remained anathema and continues to be harassed by uninformed quantum chemists even to these days. And all this despite a Pleiades of the supporters of Mathematical Chemistry and Chemical Graph Theory. They include: Jerome Karle,^{43,44} Robert G. Parr, Roald Hoffmann, Sir Harry Kroto, Rudolf Marcus, Dudley Herschbach, Ahmed Zewail, Alan Kartritzky, Alexandru T. Balaban and other outstanding Honorary Fellows of The International Academy of Mathematical Chemistry.⁴⁴ Thus Mathematical Chemistry and Chemical Graph Theory are still waiting the day of deserving recognition despite unproductive obstructions by misguided entrenched quantum chemists.

The fact that the same scientific discipline, the Theoretical Chemistry, is associated with two “historical blunders,” the Density Functional Theory and the Chemical Graph Theory, is significant indicator that “Something is rotten in the state of Denmark.” However, this need not be surprising and unexpected in view of an observation of O. J. Hirschfelder⁴⁵ stated over 25 years ago:

“Unfortunately, now there are too few theoretical chemists with sufficient vision to take a giant step of exploring completely new techniques. Instead, scientists in the

1980s get so immersed in a maze of computational detail that they lose sight of the simple, elegant theories.”

Nothing much has changed during the past 25 years that would require revision of the statement of Hirschfelder. The scientists in the 2000s remain so immersed in a maze of computational detail that they continue to lose sight of the simple, elegant theories.

Let us not forget a statement of Niels Bohr⁴⁶

“If you have a correct statement, then the opposite of a correct statement is of course an incorrect statement, a wrong statement. But when you have a deep truth, then the opposite of the deep truth may again be deep truth.”

One may say that Quantum Theory is one deep truth, that Graph Theory is another deep truth, which even are not opposing one another, yet some continue to preach only half of the truth.

An “explanation” for the above may parallel E. Bright Wilson’s observation, to be found on the introductory pages of his *“Introduction to Scientific Research”*,⁴⁷ that to appreciate “new directions” and novel approaches in science may require more imagination – a commodity that is not necessarily abundant among scientists. According to E. B. Wilson:

“The most rewarding work (in science) is usually to explore a hitherto untouched field. These are not easy to find today. However, every once in a while some new theory or new experimental method or apparatus makes it possible to enter a new domain. Sometimes it is obvious to all that this opportunity has arisen, but in other cases recognition of the opportunity requires more imagination . . . it is almost always worthwhile to explore a region which is really new. Unexpected results can generally be relied upon under these circumstances.”

POSITRONIUM

Positronium consists of an electron and positron (antiparticle to electron, which is analogous to proton, except for the mass, which equals that of electron). Positron and electron are bound together to form positronium. Because of the reduced mass the spectral frequencies of positronium are half of those of hydrogen atom. Stjepan Mohorovičić predicted the existence of positronium in 1934.¹ Experimentally it was established by Martin Deutch, at MIT in 1951,⁴⁸ who was among first to point out on the difference between orto-positronium, with parallel spins of positron and electron (³S₀ triplet ground state) with half-life of 142 nanoseconds (10⁻⁹ seconds) and para-positronium with antiparallel spins of positron and electron (¹S₀ singlet ground state) with half-life of

125 picoseconds (10⁻¹² seconds), about thousand times shorter half-life.

We would like also to add, what seems to be often overlooked, that Stjepan Mohorovičić not only calculated the spectrum of positronium, but also was actually searching for positronium spectral lines in stellar spectra, unfortunately without success. A successful identification of positronium Lyman- α radiation Ly α λ 2430 line has been the first time observed in a laboratory in 1975 by Canter and collaborators.⁴⁹ Despite half a dozen unsuccessful attempts to locate positronium de-excitation lines in the sky finally ten years later, in 1984, and 50 years after the attempts of S. Mohorovičić to detect positronium lines, McClintock⁵⁰ observed Ly α λ 2430 line in spectra of Crab Nebula. Crab Nebula, in the constellation of Taurus, which is some 6500 light years away, was known to Chinese and Arab astronomers since 11th century and was rediscovered in the western world by John Bevis, an English doctor and astronomer in 1731.

POSITRONIUM “MOLECULE”

Positronium (Ps) has been reported as being part of positronium hydride PsH, a molecule half way between hydrogen molecule (H₂) and positronium molecule Ps₂. PsH has been first predicted already in 1951 by A. Ore,⁵¹ has been observed in 1990⁵² and finally in 1992 its formation was reported by Schrader and coworker.⁵³ Very recently, less than a year ago, the production of molecular positronium, Ps₂ molecule, a system consisting of two electrons and two positrons, fully analogous to the hydrogen molecule H₂, except for the differences in mass between protons and electrons, has been reported by Cassidy and Mills.¹⁴ It is interesting that already in 1946 the existence of molecular positronium was speculated by Usukura *et al.*,^{54,55} but it took over 60 years for experimental confirmation of the speculation, for experimental proof of the existence of molecular positronium Ps₂. In contrast the experimental confirmation of positronium, the work of M. Deutsch,⁴⁸ took “only” 17 years of “waiting.” One may say that the “Waiting for Godot,” both for Ps and Ps₂, though it took time, in contrast to Samuel Beckett’s play⁵⁶ eventually paid off.

SPECULATIONS

Positronium started as a speculation so it seems fitting to end this article, the heart of which is positronium, with speculations. Having positronium Ps, positronium hydride PsH, and “molecular” positronium Ps₂ one may ask: What next? Well in view of the quadrupling of the

“waiting period” from Ps to Ps₂ for arrival of Godot, it may be safe, even for younger scientists, to speculate “impossible.” How about, for instance, a speculation about the “Ps⁺” and analog of H₂⁺ and “Ps⁻”. There is, however, a significant difference between molecular hydrogen and molecular hydrogen ion on one side, and the corresponding Ps₂ and Ps⁺. Hydrogen ion, H₂⁺, represents the simplest quantum chemical system, a molecule having a single electron. The hydrogen molecule H₂, a two electron system, is computationally very much more involved, as demonstrated by Kołos and Wolniewicz in 1965,⁵⁷ who were calculating very accurate potential energy curves for the ground state and two excited states. Of course, the H₂⁻ is computationally even more involved as it involves the interactions of three electrons.

In case of positronium ions, Ps⁺ and Ps⁻, one has the problem of “three particles” of different charge and equal mass. Incidentally, from the computational point of view the two ions, the positive and the negative, are fully equivalent. One can continue to speculate about positronium “molecular” ions that would be analogous to higher members of small hydrogen molecular ions H₂⁺, the H_n⁺,⁵⁸⁻⁶¹ but instead of consisting of protons and electrons they would consist of various numbers of positrons and electrons. There may be no end to speculations, and while hypothetical non-bond positronium “molecular” ions may be elusive, experimentally and computationally, at least for a while, positronium appears to be not so rare, as it may have been thought in the recent past.

Before ending and instead of apology for the rambling speculations recall the statement of M. Klotz:⁶²

“Some eccentric ideas in science seem immortal. They do not die; they do not even fade away. They merely lie dormant, or submerged in the collective scientific subconscious, and are revived often in a slightly different guise.”

Let us be composed and dispassionate: It is better to solve a small part of an important problem, than to speculate about “impossible,” but on the other hand it is better to speculate “impossible” than completely solve an unimportant problem.

Unfortunately it appears that there are plenty of scientists considering issues of problematic importance rather than paying attention to unusual and unfamiliar, strange and odd, irregular and atypical, unexpected and unconventional, different and uncommon. Many ideas in science, small and large, may appear eccentric to many and even most, but what matters is that they appear central to few. Recall how the publication of van't Hoff “The arrangement of atoms in space” was “greeted” by one of the leading German organic chemists, Hermann

Kolbe, when van't Hoff with Le Bell announced the hypothesis of the tetrahedral carbon atom. Kolbe⁶³ in *Journal für praktische Chemie* (of which he was the editor) has referred to van't Hoff as one of

“... pseudoscientists from junk-room which harbor such failing of human mind, and is dressed up in modern fashion and rouged freshly like a whore whom one tries to smuggle into good society where she does not belong.”

Let us list some ideas in science of interest in Theoretical Chemistry that may appear eccentric to many and some of which were greeted with the same lack of enthusiasm for novelty that permeate Kolbe's view on “Imagination in Science” (which was the title of van't Hoff's Nobel Prize lecture). Here is a collection for the start:

Hormesis,^{23,24,38} Density Functional Theory,^{39,40} Chemical Graph Theory,^{64,65} Buckminsterfullerene,¹⁵ Bullvalene,¹⁶ Clar's aromatic sextet,⁶⁶ Degenerate rearrangement graphs,⁶⁷ Conjugated circuits,^{68,69} Canonical Labels,^{70,71} Chaos game,⁷² Representation of DNA by chaos game,⁷³ Virtual genetic code,⁷⁴ Retro-regression,⁷⁵ Wiener index,⁷⁶ Hosoya topological index,⁷⁷ The connectivity index,⁷⁸ Numerical Kekulé valence structures,^{69,79} Resistance distance,⁸⁰ Periodic Table of Isomers,^{81,82} Graphical representation of DNA,⁸³ Spectral representation of DNA,⁸⁴ Graphical representation of proteins by star-like graphs,⁸⁵ Variable connectivity index,⁸⁶ 8x8 Table of Codons,⁸⁷ Graphical alignment of DNA,⁸⁸ Graphical alignment of proteins⁸⁹ – all these and many other ideas are illustrations of “eccentric” ideas to some and “central” to others.

Coming back to Stjepan Mohorovičić and positronium we may summarize the situation by quoting E. Bright Wilson,⁴⁷ who wrote:

“Many scientists owe their greatness not to their skill in solving problems but to their wisdom in choosing them.”

Recall that calculating energy levels of hydrogen and thus of positronium is fairly straightforward, if not simple, but the greatness of Stjepan Mohorovičić is in his vision, in “choosing the problem” involving matter-antimatter, only one year after Anderson detected experimentally positron,⁹⁰ and several years after Dirac⁹¹ postulated the existence of positron! What interested Stjepan Mohorovičić is what happens when electron and positron are passing close enough to be attracted by Coulomb forces – and the answer was positronium! A Nobel Prize to Stjepan Mohorovičić and Martin Deutsch would be a recognition of chemistry of “atoms” and “molecules” that have no nuclei – a novelty in Chemistry of considerable latitude.

Acknowledgements. I wish to thank Dr. S. Bosanac, the Director of the Brijuni Conference “Hydrogen: A universal saga” (25-29 August 2008), for allowing presentation of my poster “Positronium – hydrogen-like and unlike” at the conference a day before the conference started. I also thank very much Academician Vladimir Paar on informative correspondence about Stjepan Mohorovičić. The last but not the least, I thank Professor Jure Zupan, Dr. Marjana Novič and Dr. Marjan Vračko, of The National Institute of Chemistry, Ljubljana, Slovenia, for their warm hospitality, understanding, and continuation of support of my annual three months research in Chemical Graph Theory, Mathematical Chemistry, and Bioinformatics, which now extends for over 15 years ago.

REFERENCES

- S. Mohorovičić, Möglichkeit neuer Elemente und ihre Bedeautung in Astrophysik. *Astron. Nachr.* **253** (1934) 94.
- H. Kragh, From “electrum” to positronium, *J. Chem. Educ.* **67** (1990) 196–197.
- H. Galič, *Priroda* 1, 1982.
- V. Paar, “Stjepan Mohorovičić – otac pozitronija,” *Hrvatski Znanstveni Zbornik*, 1993.
- V. Glaser, *Kovarijantna kvantna elektrodinamika*, Zagreb (1955).
- J. Schwinger (Ed.), *Selected papers on Quantum Electrodynamics*, Dover Publications, New York, 1958.
- R. P. Feynman, *Quantum Electrodynamics: The Strange Theory of Light and Matter*.
- D. C. Kennedy (2000), arXiv:astro-ph/0003485v2
- G. Gabrielse, D. S. Hall, T. Roach, P. Yesley, A. Khabbay, J. Estrada, C. Heinmann, and H. Kalinowsky, *The ingredients in cold antihydrogen: Simultaneous confinement of antiproton and positrons as 4K*. *Phys. Lett. B* **455** (1999) 311–315.
- G. Andersen, W. Bertsche, A. Boston, P. D. Bowe, C. L. Cesar, S. Chapman, M. Charlton, M. Chartier, A. Deutsch, J. Fajans, M. C. Fujiwara, R. Funakoshi, D. R. Gill, K. Gomboroff, J. S. Hangst, R. S. Hayano, R. Hydomako, M. J. Jenkins, L. V. Jørgensen, L. Kurchaninov, N. Madsen, P. Nolan, K. Olchanski, A. Olin, A. Povilus, F. Robicheaux, E. Sarid, D. M. Silveira, J. W. Storey, H. H. Telle, R. I. Thompson, D. P. van der Werf, J. S. Wurtele, and Y. Yamazaki, Antimatter plasmas in multipole trap for antihydrogen. *Phys. Rev. Lett.* **98** (2007) Doi: 10.1103/98.023402
- E. A. Hessels, *Process for the production of antihydrogen*. US patent 6163587
- M. A. Monge, R. Pareja, and G. Gonzáles, Positron bound states on hydride ions in thermochemically reduced MgO single crystal, *Phys. Rev. B* **54** (1996) 8950–8953.
- G. G. Ryzhikh and J. Mitroy, The binding of positronium to lithium, *J. Phys. B, At. Mol. Opt. Phys.* **31** (1998) L103–L107.
- D. B. Cassidy and A. P. Mills, Jr., The production of molecular positronium, *Nature* **449** (2007) 195–197.
- H. W. Kroto, J. R. Heath, S. C. O’Brien, F. F. Curl, and R. E. Smalley, C₆₀, Buckminsterfullerene, *Nature* **318** (1985) 162–163.
- W. von E. Doering and W. Roth, *Tetrahedron* **19** (1963) 715.
- G. Schröder, *Angew. Chem. Int. Ed. Eng.* **2** (1963), p. 481.
- J. F. M. Oth, K. Müllen, J.-M. Gilles, and G. Schröder, Comparison of ¹³C- and ¹H-magnetic resonance spectroscopy as techniques for the quantitative investigation of dynamic processes. The Cope rearrangement in bullvalene. *Helv. Chim. Acta* **57** (1974), 1415.
- M. Randić, D. O. Oakland, and D. J. Klein, Symmetry properties of chemical graphs. IX. The valence tautomerism in the P₇³⁻ skeleton. *J. Comput. Chem.* **7** (1986) 35–54.
- J. Brocas, The reaction graph of the Cope rearrangement in bullvalene, *J. Math. Chem.* **15** (1994) 389–395.
- M. H. Klin, S. S. Tratch, and N. S. Zefirov, Group-theoretical approach to the investigation of reaction graphs for highly degenerate rearrangements of chemical compounds. *J. Math. Chem.* **7** (1991) 135–151.
- T. Živković, Bullvalene Reaction Graph, *Croat. Chem. Acta* **69** (1996) 215–222.
- E. J. Calabrese, Historical blunders: how toxicology got the dose-response relationship half right. *Cell Mol. Biol.* **51** (2005) 643–654.
- E. J. Calabrese, Paradigm lost, paradigm found: the re-emergence of hormesis as a fundamental dose response model in the toxicological sciences. *Environ. Pollut.* **138** (2005) 379–411.
- M. Randić, On graphical and numerical characterization of proteomics maps. *J. Chem. Inf. Comput. Sci.* **41** (2001) 1330–1338.
- M. Randić, J. Zupan, and M. Novič, On 3-D graphical representation on proteomics maps and their numerical characterization. *J. Chem. Inf. Comput. Sci.* **41** (2001) 1339–1344.
- M. Randić, F. Witzmann, M. Vračko, and S. C. Basak, On characterization of proteomics maps and chemically induced changes in proteomes using matrix invariants: application to peroxisome proliferators. *Med. Chem. Res.* **10** (2001) 456–479.
- M. Randić, M. Novič, and M. Vračko, On characterization of dose variations of 2-D proteomics maps by matrix invariants. *J. Proteome Res.* **1** (2002) 217–226.
- M. Randić and S. C. Basak, A comparative study of proteomics maps using graph theoretical biodescriptors. *J. Chem. Inf. Comput. Sci.* **42** (2002) 983–992.
- M. Randić, A graph theoretical characterization of proteomics maps. *Int. J. Quantum Chem.* **90** (2002) 848–858.
- M. Randić, J. Zupan, M. Novič, B. D. Gute, and S. C. Basak, Novel matrix invariants for characterization of changes of proteomics maps, *SAR & QSAR in Environ. Res.* **15** (2004) 147–157.
- M. Randić, Quantitative characterization of proteomics maps by matrix invariants in: P. M. Conn (Ed.), *Handbook of Proteomics Methods*, Human Press, Inc. Totowa, NJ (2003) pp. 429–450.
- Ž. Bajzer, M. Randić, D. Plavšić, and S. C. Basak, Novel map descriptors for characterization of toxic effects in proteomics maps. *J. Mol. Graphics & Modelling* **22** (2003) 1–9.
- M. Randić, N. Lerš, D. Vukičević, D. Plavšić, B. D. Gute, and S. C. Basak, Canonical Labeling of Proteome Maps. *J. Proteome Res.* **4** (2005) 1347–1352.
- M. Randić, N. Novič, and M. Vračko, Novel characterization of proteomics maps by sequential neighborhood of protein spots. *J. Chem. Inf. and Modeling* **45** (2005) 1205–1213.
- M. Randić, F. A. Witzmann, V. Kodali, and S. C. Basak, Dependence of a characterization of proteomics maps on the number of protein spots considered. *J. Chem. Inf. Model.* **46** (2006) 116–122.
- M. Randić, Quantitative characterization of proteome: Dependence on the number of proteins considered, *J. Proteome Res.* **5** (2006) 1575–1579.
- M. Randić and E. Estrada, Order from chaos: Observing hormesis at the proteome level. *J. Proteome Res.* **4** (2005) 2133–2136.
- R. G. Parr and W. Yang, *Density Functional Theory of Atoms and Molecules*, Oxford Univ. Press, New York, 1989.
- N. H. March, *Electron Density Theory of Atoms and Molecules*, Academic Press, 1992.
- See a letter of Professor R. G. Parr to this author (February 28, 2004) reproduced on pp. 112–113 in ref. [42].

42. M. Randić, On history of the Randić index and emerging hostility toward Chemical Graph Theory, *MATCH Commun. Math. Comput. Chem.* **59** (2008) 5–124.
43. See a letter of Jerome Karle to this author at the occasion of initiation of The International Academy of Mathematical Chemistry, available at web.
44. The International Academy of Mathematical Chemistry, with seat in Dubrovnik, Croatia, was established in 2005, at its first meeting, in the city of Dubrovnik on Adriatic (Croatia). It promotes application of mathematics beyond Calculus, in particular the discrete mathematics, to chemistry. It is a counterpart to The International Academy of Quantum Science, with seat in Menton, on Mediterranean sea, France, founded in 1967 and covering applications of quantum theory to chemistry and chemical physics.
45. O. J. Hirschfelder, *Ann. Rev. Phys. Chem.* **34** (1983) 1.
46. A statement of Werner Heisenberg attributed to Niels Bohr: Heisenberg, W. Theory, Criticism and Philosophy. A chapter in: Lifshitz, E. M. From a Life of Physics, World Scientific Co. Singapore, 1989, p. 55.
47. E. B. Wilson, *Introduction to Scientific Research*, Mc Graw-Hill.
48. M. Deutsch, *Phys. Rev.* **82** (1951) 455.
49. K. F. Canter, A. P. Mills, and S. Berko, Observations of positronium Lyman- α radiation, *Phys. Rev. Lett.* **34** (1975) 177–180 (Erratum: *Phys. Rev. Lett.* **34** (1975) 848).
50. J. E. McClintock, Detection of positrons via the optical lines positronium. *Astrophys. J.* **282** (1984) 1.
51. A. Ore, The existence of Wheeler-compounds. *Phys. Rev.* **83** (1951) 665–665.
52. R. Peraja and R. Gonzales as cited in Wikipedia under “Positronium hydride.”
53. D. M. Schrader, F. M. Jacobsen, N-P. Frandsen, and U. Mikkelsen, Formation of positronium hydride, *Phys. Rev. Lett.* **69** (1992) 57–60.
54. J. Usukura, K. Varga, and Y. Suzuki, Signature of the existence of the positronium molecule. *Phys. Rev. A* **58** (1998) 1918–1931.
55. J. Wheeler as cited in ref. [54].
56. S. Beckett, *Waiting for Godot*, Faber and Faber, London: 1956.
57. W. Kołos and L. Wolniewicz, Potential-energy curves for their $X^1\Sigma_g + b^3\Sigma_u$, and $C^1\Pi_u$ states of hydrogen molecule, *J. Chem. Phys.* **43** (1965) 2429–2441.
58. L. P. Viegas, A. Alijah, and A. J. C. Varandas, *J. Chem. Phys.* **126** (2007).
59. A. Alijah and A. J. C. Varandas, *Phil. Trans. Roy. Soc. A* **364** (2006) 2889.
60. T. Mendes Ferreira, A. Alijah, and A. C. J. Varandas, *J. Chem. Phys.* **128** (2008).
61. A. Alijah, Recent progress on small hydrogen molecular ions, Abstract Book, Brijuni Conference XI: *Hydrogen: A Universal Saga*. Brijuni, Croatia, 25–29 Sept. 2008, p. 13.
62. I. M. Klotz, *The Mathematicker Intelligenzer* **17** (1995) 46.
63. J. H. van't Hoff, *Imagination in Science*, Springer Verlag: Berlin (1967).
64. N. Trinajstić, *Chemical Graph Theory*, CRC Press, Boca Raton, FL 1992.
65. D. Bonchev and D. H. Rouvray (Eds.): *Chemical Graph Theory: Introduction and Fundamentals*, ISBN 0856264547.
66. E. Clar, *The Aromatic Sextet*, Wiley, London, 1972.
67. A. T. Balaban, D. Farcasiu, and R. Banica, Graphs of multiple 1,2-shifts in carbonium ions and related systems. I *Revue Roumaine de Chimie* **11** (1966) 1205.
68. M. Randić, Conjugated circuits and resonance energies of benzenoid hydrocarbons. *Chem. Phys. Lett.* **38** (1976) 68–70.
69. M. Randić, Aromaticity of polycyclic conjugated hydrocarbons. *Chem. Rev.* **103** (2003) 3449–3605.
70. M. Randić, On the recognition of identical graphs representing molecular topology. *J. Chem. Phys.* **60** (1974) 3920–3928.
71. M. Randić, On canonical numbering of atoms in a molecule and graph isomorphism. *J. Chem. Inf. Comput. Sci.* **17** (1977) 171–180.
72. M. F. Barnsley and H. Rising, *Fractals Everywhere*, 2nd ed. Boston, MA: Academic Press, 1993.
73. H. I. Jeffrey, Chaos game representation of gene structure. *Nucleic Acid Res.* **18** (1990) 2163–2170.
74. M. Randić, 2-D graphical representation of proteins based on virtual genetic code. *SAR & QSAR in Environ. Res.* **15** (2004) 147–157.
75. M. Randić, Retro-regression – another important multivariate regression improvement. *J. Chem. Inf. Comput. Sci.* **41** (2001) 602–606.
76. H. Wiener, Structural determination of paraffin boiling points. *J. Am. Chem. Soc.* **69** (1947) 17–20.
77. H. Hosoya, Topological index. A newly proposed quantity characterizing topological nature of structural isomers of saturated hydrocarbons. *Bull. Chem. Soc. Jpn.* **44** (1971) 2332–2339.
78. M. Randić, Characterization of molecular branching. *J. Am. Chem. Soc.* **97** (1975) 6609–6615.
79. M. Randić, Algebraic Kekulé formulas for benzenoid hydrocarbons. *J. Chem. Inf. Comput. Sci.* **44** (2004) 365–372.
80. D. J. Klein and M. Randić, Resistance distance. *J. Math. Chem.* **12** (1993) 81–95.
81. M. Randić and C. L. Wilkins, On a graph theoretical basis for ordering of structures. *Chem. Phys. Lett.* **63** (1979) 332–336.
82. M. Randić and C. L. Wilkins, Graph theoretical ordering of structures as basis for systematic searches for regularities in molecular data. *J. Phys. Chem.* **83** (1979) 1525–1540.
83. E. Hamori and J. Ruskin, H curves, a novel method of representation of nucleotide series especially suited for long DNA sequences. *J. Biol. Chem.* **285** (1983) 1318–1327.
84. M. Randić, M. Vračko, N. Lerš, and D. Plavšić, Novel 2-D graphical representation of DNA sequences and their numerical characterization. *Chem. Phys. Lett.* **368** (2003) 1–6.
85. M. Randić, J. Zupan, and D. Vikić-Topić, Graphical representation of proteins by star-like graphs. *J. Mol. Graphics & Modelling* **26** (2007) 290–305.
86. M. Randić, Novel graph theoretical approach to heteroatom in quantitative structure-activity relationship. *Intel. Lab. Syst.* **10** (1991) 213–227.
87. M. Randić, J. Zupan, and A. T. Balaban, Unique graphical representation of protein sequences based on nucleotide triplet codons. *Chem. Phys. Lett.* **397** (2004) 247–252.
88. M. Randić, J. Zupan, D. Vikić-Topić, and D. Plavšić, A novel unexpected use of a graphical representation of DNA: Graphical alignment of DNA sequences. *Chem. Phys. Lett.* **431** (2006) 375–379.
89. M. Randić, On a geometry-based approach to protein sequence alignment. *J. Math. Chem.* **43** (2008) 756–772.
90. C. D. Anderson, The positive electron, *Phys. Rev.* **43** (1933) 491–494.
91. P. A. M. Dirac, The quantum theory of electron, *Proc. Roy. Soc (London) A* **117** (1928) 610–612.

SAŽETAK**Positronium – Sličan vodik i različit****Milan Randić***National Institute of Chemistry, Ljubljana, Slovenia*

Dan je kraći revijski prikaz positroniuma, Ps, (sustav podoban atomu vodika, koji je međutim gradjen od elektrona i pozitrona), od njegovog početka 1935 godine do najnovijih rezultata, positronium hidrida PsH i positronium molecule. Kako je pokazao Stjepan Mohorovičić positronium predstavlja relativno stabilno sustav materije i antimaterije. Mohorovičić je izračunao spektar positroniuma i što više, tražio Lyman- α zračenje u spektrima zvijezda. Prošlo je 40 godina do eksperimentalne observacije linije Ly α 12430 u laboratoriju Cantera i suradnika 1975 godine. Još je proteklo 10 godina do astronomske observacije positroniumovih linija 1984 godine u nebuli raka. Rad Stjepana Mohorovičića je ponajviše ignoriran u njegovoj rodnoj Hrvatskoj sve do najnovijih dana, ilustracija “povjesne zablude” lokalnih fizičara – fenomen koji nije nepoznat u znanosti općenito, kao što je nedavno ilustrirano širom svijeta s okljevanjem prihvaćanja nelinearnog odgovora organizma o ovisnosti o koncentraciji doze (hormesa); ovisnosti svojstva više-elektronskih sustava o prostornoj raspodjeli elektronske gustoće (DFT); i kemijske teorije grafava.