

Hadronic Chemistry and Binding Energies¹

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Abstract. In this short paper we have briefly reviewed the valence bond treatment of Santilli based on *isoelectronium* and his iso-mathematics. It is now known as hadronic chemistry. We have discussed the cases of hydrogen, water and magneclules with the emphasis on their energetics. We have taken this opportunity to re-examine Eyring's transition state theory based assertion of a shallow minima at the top of the barrier for bimolecular chemical reactions by juxtaposing the *isoelectronium* of two electrons in a singlet state to the requirement of three electron bonding of the activated complex. The preliminary answer is in negation of any stability of activated complex.

Keywords: Hadronic Chemistry, Isochemical Models, Binding Energy, Magneclules, Hydrogen molecule, Water Molecule

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INTRODUCTION

The quantum mechanical calculations of binding energies of neutral molecules by different methods have always fascinated chemists and physicists across the globe. The most commonly used are the variation and perturbation methods [1, 2]. The perturbation method uses the solution for energy of zero order systems to find a solution for the required system in hand. Whereas, the variation method consists of Linear Combination of Atomic Orbitals (LCAO) to generate Molecular Orbitals (MO). Hence it is also referred as LCAO-MO theory or in short MO theory. Other notable variant of variation method is the Self-consistent Field (SCF) theory. These variation methods involve approximations and as a result of this the binding energies so obtained do not accurately match with the experimental values [1, 2]. The energy calculated for H₂ molecule by LCAO-MO method is observed to be -1.0985 a.u. (Binding energy = - 2.681 eV) as against the experimental value of -1.174 a.u. (Binding energy = - 4.75 eV). By applying the valence-bond (VB) theory (Hitler-London) [3] the value for energy is observed to be -1.1160 a.u. (Binding energy = -3.140 eV). Thus apparently it is observed that the VB method is better than MO theory but this conclusion is not justified as both are gross approximations to the actual state of affairs in the molecule. One of the great shortcomings of the MO theory is that the ionic terms enter into the wave function with the same weight as nonionic terms. In VB theory the wave function consists of the covalent part only. Thus, a conclusion can be drawn that it is better to leave altogether the ionic terms out of the wave functions for Hydrogen molecule.

In the light of above facts Professor Santilli opined that the fundamental quantum chemical notion of valence bond as presented in the 20th century literature is pure nomenclature without any quantitative scientific content because to be quantitative the preceding notion should,

1. identify clearly the force between two identical valence electrons,
2. prove that such a force is attractive as an evident necessary prerequisite to claim the sufficiently strong bond needed for molecule formation, and

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3. prove that such a clearly identified and clearly attractive force verifies indeed the experimental data on molecular structures.

Thus, it is impossible for quantum chemistry to meet the above conditions because in quantum mechanics one uses the Coulomb law to describe the interactions between two identical electrons that obviously maintains that the two identical electrons must repel each other and certainly they cannot attract each other.

Santilli never accepted these notions of so-called well established theory of quantum chemistry. His untiring efforts of a few decades gave birth to the new discipline of Hadronic Chemistry [4]. Hadronic chemistry of small molecules is based on Santilli's iso- and geno- mathematics by considering the interactions at 10^{-15} m or less [4–6]. The main idea is that at such short distances the wave packets of electrons lose their point like character considered at atomic distances rather they overlap each other considerably (see Figure 1).

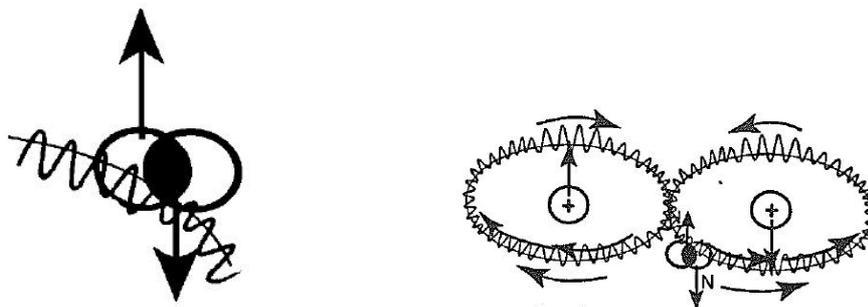


FIGURE 1. (a) In the left Figure: Schematic representation of the deep overlapping of the wavepackets of the valence electrons in singlet coupling (that meets the Pauli exclusion principle). These conditions are known to be nonlinear, nonlocal and nonpotential (due to the zero-range contact interactions), thus not possible to be represented via Hamiltonian and consequently not being unitary. As a result, the ultimate nature of the valence bonds is outside any credible representation via quantum chemistry. The Hadronic Chemistry has been built for the specific scope of representing the conditions considered herein of the bonding valence electrons. (b) In the right Figure: Schematic representation of *Isochemical model* of Hydrogen Molecule showing oo shaped orbit of *isoelectronium*

The present study is aimed at reviewing energetics of H_2 , H_2O and a representative magneuclear species using the methods of Hadronic Chemistry.

SANTILLI AND SHILLADY MODEL FOR HYDROGEN MOLECULE

Santilli and Shillady in their historical paper [7] of 1999 proposed a model of H_2 molecule and produced the concept of isoelectronium for stable quasidelectron singlet state (see Figure 1) that enabled exact solution of Santilli-Schrödinger equation. In the said paper they considered that the electrons have extended wave packets of the order of 10^{-15} m, whose mutual penetration as necessary for valence bond, causes non-linear, non-local and non-potential interactions is at the very foundations of hadronic mechanics. They introduced the following realization of a non-unitary transform that is the fundamental isounit of hadronic chemistry,

$$UU^\dagger = \hat{I} = \frac{1}{T} = \exp\left([\psi(r)/\hat{\psi}(r)] \int \psi_1^\dagger(r)\psi_2(r)d^3r\right) = 1 + [\psi(r)/\hat{\psi}(r)] \int \psi_1^\dagger(r)\psi_2(r)d^3r + \dots \quad (1)$$

where ψ and $\hat{\psi}$ are the solutions of unitary and non-unitary Schrödinger equations respectively and ψ_k , $k = 1, 2, \dots$ are the conventional quantum mechanical wave functions of the two electrons.

They began with the nonrelativistic quantum mechanical equation of two electrons in singlet coupling and then transformed it into the *isoelectronium* representation. This transformation is depicted below,

$$\left(\frac{p^2}{m} + \frac{e^2}{r}\right) \psi(r) = E\psi(r) \quad \longrightarrow \quad \left[\frac{p_{isoelec}^2}{2m_{isoelec}} - V' \frac{e^{-br}}{1 - e^{-br}}\right] \hat{\psi}(r) = E'\hat{\psi}(r), \quad (2)$$

where, m is electron mass, $m_{isoelec}$ and $p_{isoelec}$ are the mass and momentum respectively of isoelectronium, and V' reflects the absorption of the repulsive coulombic potential by the much stronger attractive Hulthén potential.

Thus, Santilli-Shillady achieved for the first time in history of chemistry a valence bond formed by two identical electrons in singlet coupling with a strongly attractive force as expected by experimental evidence which is known as Santilli - Shillady strong valence bond and hence it correctly describes that the H₂ molecule is not paramagnetic.

Conventionally the Hydrogen molecule is a *four body system* (two protons and two electrons). However, with the advent of *isoelectronium model* it gets reduced to a *three body system*. Its final representation with nonunitary transform reads as [4–6],

$$\left[\frac{p_{isoelec}^2}{2m_{isoelec}} + \frac{p_a^2}{2m_{prot}} + \frac{p_b^2}{2m_{prot}} - V' \frac{e^{-br}}{1 - e^{-br}} + \frac{e^2}{R} \right] \psi(r) = E' \psi(r) \quad (3)$$

where m_{prot} is the mass of proton and p_a and p_b are the momenta of protons. The above equation is purely quantum mechanical because all distances between constituents are much bigger than 1 fm. An exact variational solution of model (3) was first studied by Aringazin and Kucherenko [8] and further its exact analytical solution was achieved by Pérez-Erínquez, Marín and Rirera [9].

The energy calculated by using this model [8, 9] was found to be -1.174474 a.u. (Binding energy = - 4.74487 eV). Thus, this is in excellent agreement with the experimental value -1.174 a.u. (Binding energy = - 4.75 eV). We have described the use of *stable isoelectronium*. For the description starting with the *unstable isoelectronium* the reader may see for example the reference [6].

SANTILLI AND SHILLADY MODEL FOR WATER MOLECULE

Subsequently in 2000, Santilli and Shillady applied their above described isochemical model to study water molecule [10]. For the water molecule we have the following experimental data [6]. The energy of formation of the water molecule from hydrogen and oxygen atoms is - 9.511 eV, the binding energy is - 10.086 eV, the dissociation energy of O-H is 5.11 eV and H alone is 4.40 eV.

Notice that in water molecule we have two *isoelectroniums* one each for two O-H bonds. Due to restrictions on the length of this paper we are giving herein only the final isoelectronium representation for one O-H bond of water molecule obtained by Santilli and Shillady [10] and in tune with eq.(3) that reads as,

$$\left[\frac{p_{isoelec}^2}{2m_{isoelec}} + \frac{p_{prot}^2}{2m_{prot}} + \frac{p_O^2}{2m_O} - V' \frac{e^{-br_{12}}}{1 - e^{-br_{12}}} - \frac{2e^2}{r_{2a}} - \frac{2e^2(1 - e^{-\alpha r_{1b}})}{r_{1b}} + \frac{e^2(1 + e^{-\alpha R})}{R} \right] \psi(r) = E' \psi(r). \quad (4)$$

where, E' is the half of the binding energy of water molecule, R is the interatomic distance, r_{12} is the distance between two electrons, r_{1b} and r_{2a} are the distances between electrons and nuclei of oxygen and proton and α is the positive parameter taking care of screening of hydrogen and oxygen nuclei. The above equation achieved the first numerically exact representation of binding energy and, electric and magnetic moments of the water molecule, and exactly solvable. From above eq.(4) the binding iso-energy is obtained as - 76.388340 a.u.

MAGNECULES

The discovery of isochemical models of H₂ and H₂O, led Santilli and coworkers to set their research goal to search for altogether new mode of bonding resulting in formation of stable clusters. In early 1998, Santilli introduced his new chemical species called magneccules, having the new magneccular bond [5]. Magneccules are novel chemical species having at least one magneccular bond. The atoms are held together by magnetic fields originating due to toroidal polarization of the atomic electron orbits. The rotation of the electrons within the toroid creates the magnetic field which is absent for the same atom with conventional spherical distribution of electron orbitals. When two such polarized atoms are sufficiently close to each other and in north-south north-south alignment, the resulting total force between the two atoms is attractive. The polarization is brought about by high magnetic field which is obtained as in the case of high voltage DC arc. Magneccules have been synthesized by Santilli and coworkers between identical or non-identical molecules. These magneccules and magniplexes have found applications as clean fuels [5].

There are a host of magneccules, magneplexes and magneclusters synthesized by Santilli and co-workers. For example, Santilli proposed that the species H₃ and O₃ have a magneccular structure of the type H₃ = (H - H) × H and O₃ = (O - O) × O namely, they comprise ordinary molecules H₂ and O₂ with valence bond (shown by -) plus a third atom with magneccular bond (shown by ×). The magneccular bonds have on an average strength of 20-25 kcal/mol [11].

POTENTIAL ENERGY AT THE TOP OF THE BARRIER OF CHEMICAL REACTIONS

In Eyring's transition state theory of bimolecular reaction rates the *transition state or activated complex* at the top of the barrier has been asserted as having a shallow minima (3.3 kcal/mol) [12]. The quantum mechanical calculations of the assumed linear transition state, H—H—H (H_3), at the top of the barrier for the reaction $H + H_2 \rightarrow H_2 + H$ has been carried out using London equation. There have been more sophisticated attempts to recalculate the potential energy of the asserted linear activated complex that claim higher level of accuracy of the results but the claim of the said shallow minima at the top of the barrier remained unchanged. However, as stated above the quantum mechanical calculations of valence bond is not commensurate with the reality and hence Santilli advented *isoelectronium* to describe a valence bond in conformity of reality. In view of this advancement in our understanding of valence bond it is a pertinent question whether there can be an *isoelectronium* counterpart for three electrons forming a weakly stable activated complex state. The answer of this question seems to be in negative and hence the claimed shallow minima at the top of the barrier turns out to be a fallacious outcome.

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