

Molecular Theory Considering Nuclear Potential Wells

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Research Article

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Molecular theory considering nuclear potential wells[□]

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□ This article is submitted in honor of Prof. Peter Politzer who admitted the author to his research group, taught, helped and supported him until he could make contributions to theoretical physical chemistry.

Abstract:

This article introduces potential wells around nuclei and their roles in chemical bonds. The approach uses one-electron Bohr atomic model concept. Multi-electron atoms are converted to one-electron atoms by grounding all inactive, non-reacting electrons using the Apparent Nuclear Charge (ANC) and Electron Shielding Effect (ESE) concepts introduced in earlier publications. Then the resulting two one-electron atoms and their potential wells are utilized to obtain the related chemical bond length. The methodology is applicable to all elements of periodic table without a need for any additional tool. To test the concept, calculated bond lengths were compared to experimental ones for about 90 different bonds which showed an average error of less than 5%. The article discusses some nontraditional views for chemical bonds which may contradict the traditional beliefs in chemistry. Hopefully, readers would consider the calculated results in support of the presented views. Attached to this article is a computer software program which was prepared with sample input and output files for readers. The software can be utilized to obtain any interested bond length. The software is applicable to all elements in the periodic table up to the element Hassium with the atomic number of 108.

Keywords: Nuclear potential wells; Location of potential wells; Depth of potential wells; Chemical bonds; Bond lengths; Molecular structure; Molecular theory; Bohr atomic model; DE Broglie's concept; Schrödinger molecular theory; Ionization Energy; Atomic Shell Structure

Introduction:

The primary objective of this article is to introduce a new approach to estimate chemical bonds within molecules. The article is a continuation of a few earlier works [1-3] as well as the previous research works of Politzer et al [4-13] to establish a better understanding of atomic and molecular structures. To better understand the concept presented in this article, a review of earlier works seems to be essential and necessary. Thus a brief review over the Bohr atomic model, De Broglie's hypothesis and the Schrödinger's molecular theory would be made before presenting the new concept.

Bohr Atomic Model [14-23]:

Niels Bohr and Ernest Rutherford atomic model presented in 1913 is a simple well-understood one-electron atomic model using classical mechanics. It assumes circular orbit for the electron in equilibrium under two forces. One force is the centripetal force acting on the electron due to its rotational speed which is assumed to be equal to the attracting coulombic force acting on electron by the nucleus (Eq.1).

$$\frac{m_e v^2}{r} = \frac{Z e^2}{4 \epsilon_0 r^2} \quad (1)$$

in which m_e is the mass of electron, v the velocity of electron, r the orbital radius, Z the nuclear charge, e the electron's charge, and finally ϵ_0 is the vacuum permittivity. Rearranging the formula would provide us with formulas for velocity and radius (Eq.2 & Eq.3).

$$v = \sqrt{\frac{Z e^2}{4 \epsilon_0 m_e r}} \quad (2)$$

$$r = \frac{Z e^2}{4 \epsilon_0 m v^2} \quad (3)$$

Now potential and kinetic energies of the electron can be calculated as (Eq.4 & Eq.5):

$$E_k = \text{Kinetic Energy} = +\frac{1}{2} m_e v^2 \quad (4)$$

$$E_p = \text{Potential Energy} = -\frac{Z e^2}{4 \epsilon_0 r} \quad (5)$$

Then total ground state energy of the one-electron system can be written as (Eq.6):

$$E_{tot} = \text{Total Energy} = E_k + E_p = -\frac{Z e^2}{8 \epsilon_0 r} = -\frac{1}{2} m_e v^2 \quad (6)$$

But we know that the total energy of one-electron atoms is equal to their ionization energy (Eq.7) which can be found experimentally. Therefore,

$$E_{tot} = \text{Ionization Energy} = E_{ioniz} \quad (7)$$

Therefore, one can experimentally find the ionization energy of any one-electron system and substitute it in the total energy equation (Eq.6) to find ground state radius, velocity of the electron, and components of energy. So as it can be seen, the Bohr Atomic Model which is a rigorous stand-alone classical approach for ground state applications did not probably need to be combined with De Broglie's hypothesis to cover the excited states. Chemistry is more about the ground state properties and do not need to get over-complicated by the application of quantum mechanics if it is not necessary. Perhaps, the urge of the scientists at the time to cover both ground state and excited states using this simple classical mechanic model was a mistake. With the involvement with De Broglie's hypothesis, this simple rigorous classical mechanic model was dragged into excited states, quantum mechanics and all of the related discussions with respect to the orbital angular momentum which made scientists to cast doubts in the model. Figure 1 presents a graphical application of Bohr Atomic Model to find all classical unknowns such as ground state orbital radius, electron velocity, kinetic and potential energies for a simple one-electron atomic model (i.e. Hydrogen) without getting involved with the excited states, De Broglie's hypothesis and the quantum mechanics.

Application of Bohr Model for the ground state Hydrogen (without the use of DeBroglie's hypothesis)

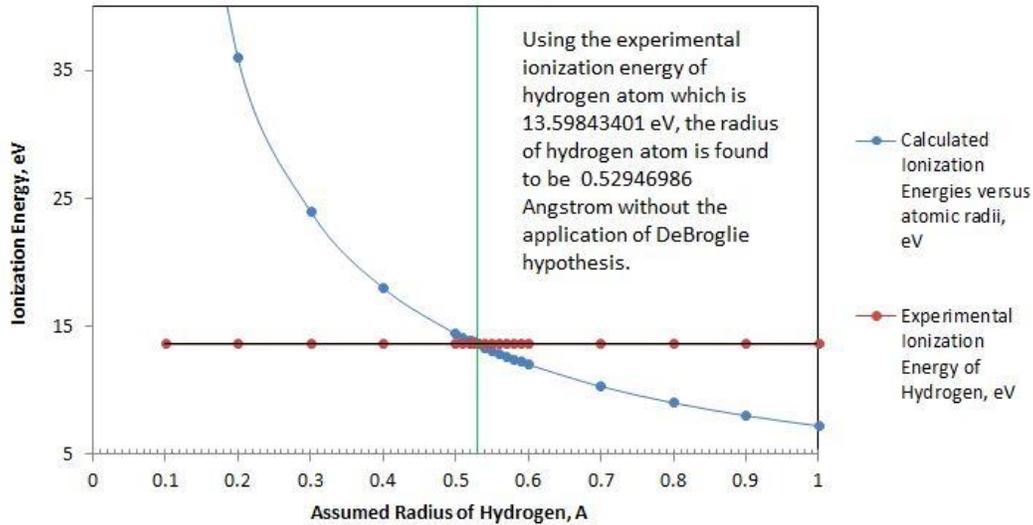


Figure 1: Graphical presentation of the application of Bohr Atomic Model

De Broglie's hypothesis [16-23]:

This postulate is considered to be the beginning, and the backbone or central part of the quantum mechanics. It states that the matter (or a particle) moves in a wave-like motion with a wavelength inversely proportional to the linear momentum of the particle (Eq.8).

$$\lambda = \frac{h}{mv} \quad (8)$$

in which λ is the wavelength of matter/particle, h the Plank's constant, m the mass of particle, and v the velocity of particle. With his postulate, it was assumed that the motion of an electron turning around the nucleus should be viewed as a standing wave. A rope constrained at both ends with a wave-like motion can get into resonance and generate whole number of wave lengths throughout its length. Similarly, the circumference of electronic orbital should be equal to a whole-number-multiplier of generated wavelengths (i.e. $2\pi r = n\lambda$). And with this thought, the following formula (Eq.9) was obtained for an atomic model which was used by Bohr in his model.

$$mvr = n \left(\frac{h}{2\pi} \right) \quad (9)$$

in which n would be a whole number such as 1, 2, 3, indicating different modes of standing wave in resonance similar to excited states. It is important to know that the wave as a motion and by itself is part of classical mechanics but in its resonance modes and jumping from one mode to another mode which generates discrete magnitudes of energy, resembles the lines observed in the atomic spectra as part of quantum mechanics.

Schrodinger's Equation [16-24]:

In 1926, Erwin Schrodinger suggested a different approach for analyzing the standing waves concept which was utilized in explanation of the dark/light lines in atomic spectra. Standing waves are called stationary states, atomic/molecular orbitals and/or energy eigenstates under different disciplines. Many developments were made later to the idea including the Hartree-Fock works [25-29], Moller-Plesset perturbation theory [30-31], and density functional theory [32-34]. Schrödinger's first step was to define electrons as waves and associating their locations with a probability density (ρ). So electrons could be anywhere with an associated probability density (Eq.10) as defined by a wave function (ψ).

$$\rho = |\psi|^2 = \psi^*(r, t) \cdot \psi(r, t) \quad (10)$$

The wave function (ψ) could take any periodic shape moving into positive, negative, and complex domains while the probability density (ρ) was always a positive value. With this definition, he broke away from classical position, orientation, and forces. Under classical mechanics, a chemical bond length could be viewed as an equilibrium position for the interacting atomic forces. Then he defined the time-independent partial differential equation governing the wave functions in stationary mode or resonance (Eq.11) as:

$$\hat{H}\psi = E\psi \quad (11)$$

in which \hat{H} is the Hamiltonian operator for kinetic and potential energies, and E the eigen values of energy. Equation (11) is an eigen value problem which would result in finding the energy states. The operator can be further written (Eq.12) as:

$$\hat{H} = \hat{T} + \hat{V}_{ne} + \hat{V}_{ee} \quad (12)$$

Where \hat{T} is the kinetic energy operator, \hat{V}_{ne} the nuclear-electron attraction potential operator, and \hat{V}_{ee} the electron-electron repulsion potential operator. The Hamiltonian can be then written in more details for a molecular bond as (Eqs.13 to 17):

$$\text{Nuclear kinetic energy} = -\frac{\hbar^2}{2} \sum_{\alpha} \frac{1}{m_{\alpha}} \nabla_{\alpha}^2 \quad (13)$$

$$\text{Electronic kinetic energy} = -\frac{\hbar^2}{2m_e} \sum_{i=1}^n \nabla_i^2 \quad (14)$$

$$\text{Nuclear repulsion potential energy} = + \sum_{\beta} \sum_{\alpha < \beta} \frac{Z_{\alpha} Z_{\beta} e^2}{4\pi\epsilon_0 r_{\alpha\beta}} \quad (15)$$

$$\text{Electronic repulsion potential energy} = + \sum_{j=2}^n \sum_{i < j} \frac{e^2}{4\pi\epsilon_0 r_{ij}} \quad (16)$$

$$\text{Nuclear - electron attraction potential energy} = - \sum_{i=1}^n \frac{Z_{\alpha} e^2}{4\pi\epsilon_0 r_{i\alpha}} \quad (17)$$

This way, the energy was only a function of electronic density and not the type and details of electron's motion or forces. The Schrödinger equation was then successfully

applied to several cases such as “Particle in box”, “Harmonic oscillator” and the “Hydrogen atom”. The application to the Hydrogen atom resulted in finding the Bohr atomic radius, and three quantum numbers of “Principal” which were shown as $n = 1, 2, 3$; and “Azimuthal” presented by $\ell = 0, 1, 2, \dots, n-1$; and the “Magnetic” quantum number shown as $m = -\ell, \dots, \ell$ for the excited states.

But the Schrödinger equation could not be solved exactly for many-electron atoms. And hence the wave function and the energy needed to be approximated. The Hartree-Fock [25-29] method provided the needed approximation method. The method is also called self-consistent field method (SCF) since the final computed field needed to be consistent with the assumed initial field. The methodology needed also an additional tool which is called “basis sets”. Basis sets [16] are in general, sets of orthogonal/orthonormal functions which are added / combined together with arbitrary or calculated coefficients to resemble a shape, a figure or a function. The belief is if we have infinite number of orthogonal functions, then by adding them together with certain coefficients, we can construct almost any figure of interest. Such a basis set is called a complete basis set (CBS). The best suggested basis set for the Schrödinger equation was the basis set formed by a finite number of the atomic orbitals found as the solutions to the hydrogen-like atoms. Those basis sets are called Slater-type orbitals (STOs). The STO orbitals decay exponentially as they get further away from the nucleus. Unfortunately, calculating integrals with STOs was computationally difficult and therefore they were substituted by Gaussian-type orbitals (GTOs). This way many basis sets such as STO-3G, STO-4G, STO-6G, STO-3G*, 3-21G, 3-21G*, 3-21G**, 3-21+G, 3-21++G, 3-21+G*, 3-21+G**, 4-21G, 4-31G, 6-21G, 6-31G, 6-31G*, 6-31+G*, 6-31G(3df, 3pd), 6-311G, 6-311G*, 6-311+G* were constructed.

Methodology:

The approach in this article does not use the Schrödinger equation to solve the multi-electron atoms participating in a chemical reaction. It uses the Bohr one-electron atomic model after grounding all inactive non-reacting electrons of the reactive atoms using ANC and ESE concepts. Once reactants are reduced to one-electron atoms, then the location of their nuclear potential wells are found and utilized to calculate the bond lengths.

Introducing the Nuclear Potential Wells:

Let's consider a Bohr-like spherical orbital with a certain radius. For example we can consider Bohr-like Hydrogen orbital with the radius of 0.52924 Å. Now let's remove the electron and instead of that place uniform distributed negative charges onto the sphere in a way that the summation of the charges placed on the sphere would add up to -1 e. Then let's find the coulombic attraction energy between the nucleus with +1 unit charge and the sphere with the distributed -1 unit charge. This potential energy would be kept as the reference value for the computation of relative potential energies. Now let's start moving the spherical orbital with the distributed charges on it away from the nucleus in a stepwise process. And in each step calculate the relative potential energy of the sphere and the nucleus which is now off-center. As the center of gravity of Bohr-like orbital

sphere moves away from the nucleus, we would see a drop in the coulombic potential energy which would continue to decrease until the center of gravity of electronic sphere arrives at 0.370468 Å distance of the nucleus. At that location which is always 70% of the Bohr radius away from the nucleus (regardless of the nuclear charge), the relative coulombic potential energy reaches at a minimum and after that point the potential energy starts increasing. Figure 2 presents the computed relative coulombic potential energy variation versus the distance between the center of gravity of electronic sphere and the nucleus.

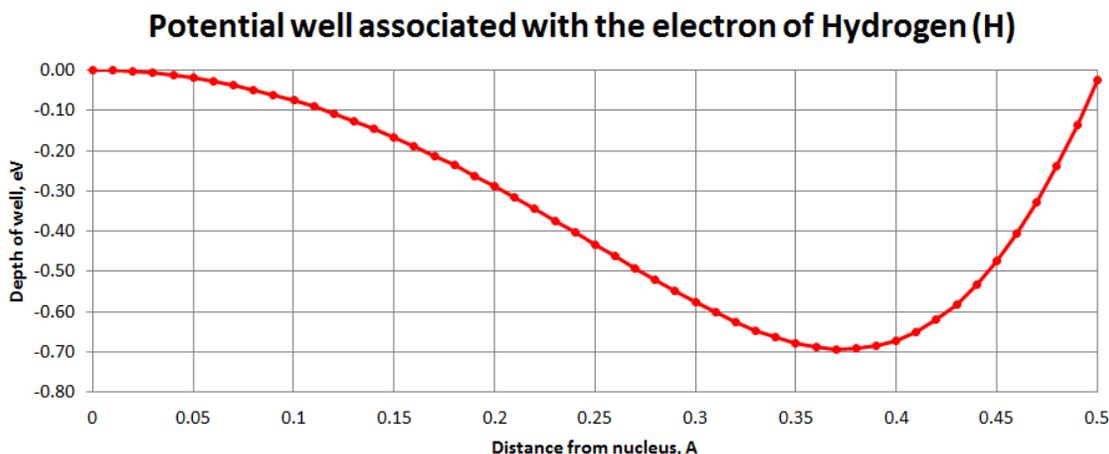


Figure 2: Nuclear potential well associated with the electron of Hydrogen atom

Similar computations were carried out for tens of other atoms which showed similar results. With multi-electron atoms, each electron was treated independently with its corresponding partial nuclear charge. This means that each time all other inactive electrons except the interested one would be grounded (or collapsed) onto nucleus in order to find the corresponding partial nuclear charge for a specific electron. The process was discussed in the previously published literatures [1-3] using two parameters of Apparent Nuclear Charge (ANC) and Electron Shielding Effect (ESE).

Once the corresponding partial charge of nucleus for each electron was found, then a computer simulation was carried out to find the location and depth of wells corresponding to each electron. To simulate the Bohr-like orbital, a sphere with the corresponding Bohr radius was segmented/grided into 32 parts. One unit electron charge was divided among those 32 segments/grids accordingly and proportional to their areas. Then a simulation was done to calculate the attractive coulombic potential energy between the segmented electroic shell and nucleus as they were separated away stepwise. Then the collected numerical data were gathered and a graph was made to pinpoint the location and depths of the wells associated with electrons. Figure 3 presents the nuclear potential wells associated with the electrons of Helium atom obtained through the same type of computation.

So under this study, it became clear that center of gravity of electrons do not remain onto the nucleus since there are wells present in vicinity of nuclei that would room the center of gravity of electrons for a lower energy. To understand this better, imagine a round rock standing at the top of a steep mountain. The rock might stay there as long as there is no

disturbance such as high winds or earthquake. But as soon as an external effect appears, the rock would roll down and would fall in a hole/well in vicinity of the peak. This is exactly what happens to electrons. The center of gravity of electrons would not stay on nuclei and they would move away and would reside in their own corresponding potential well. One may question the energy associated with the depth of well. The author believes that the energy associated with the depth of well is part atomic energy and a component of that energy. So the center of gravity of electron moves into the well and with that there should be a relaxation and redistribution of different types of atomic energy in a way that the total atomic energy would stay the same.

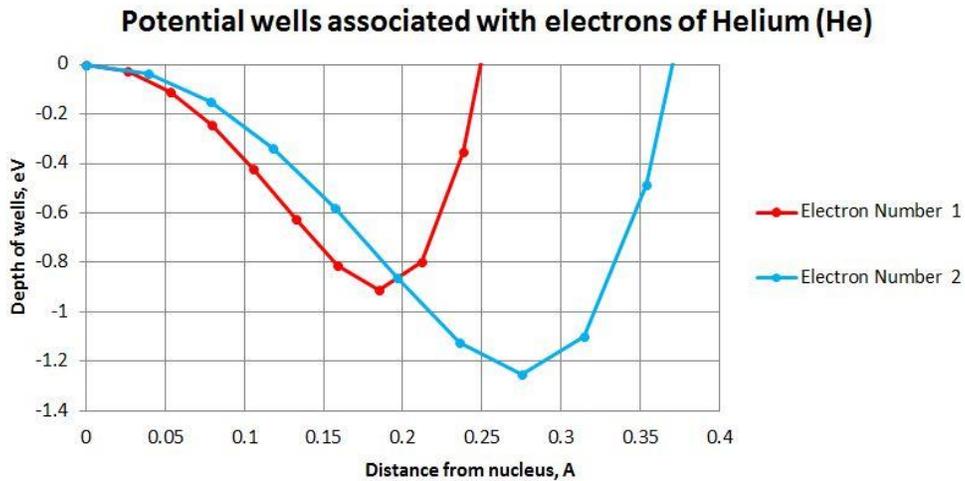


Figure 3: Nuclear potential wells associated with the electrons of Helium atom

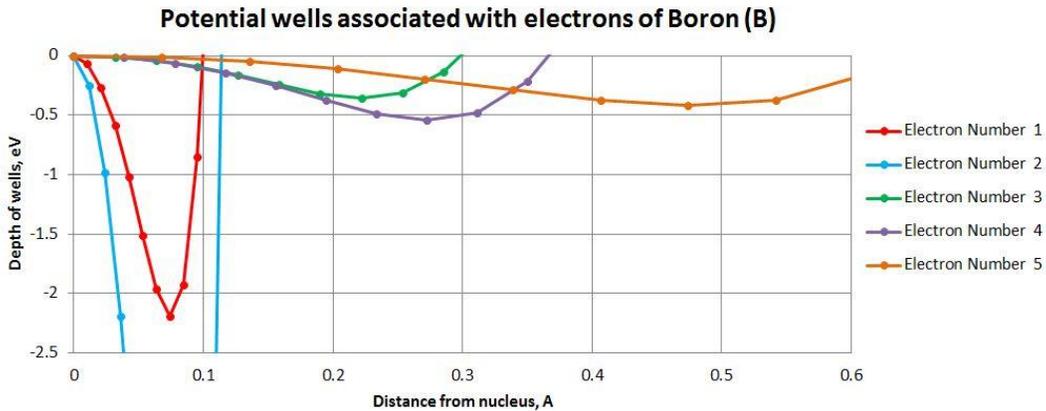


Figure 4: Nuclear potential well associated with the electrons of Boron atom

Figure 4 presents the five wells associated with electrons of Boron. As one may notice, the first two wells which associate with the s orbital of the atom are closer to the nucleus and their depths are much more compared to the other three electrons. The wells associated with the three valence electrons of Boron are located further away from the nucleus and are shallow.

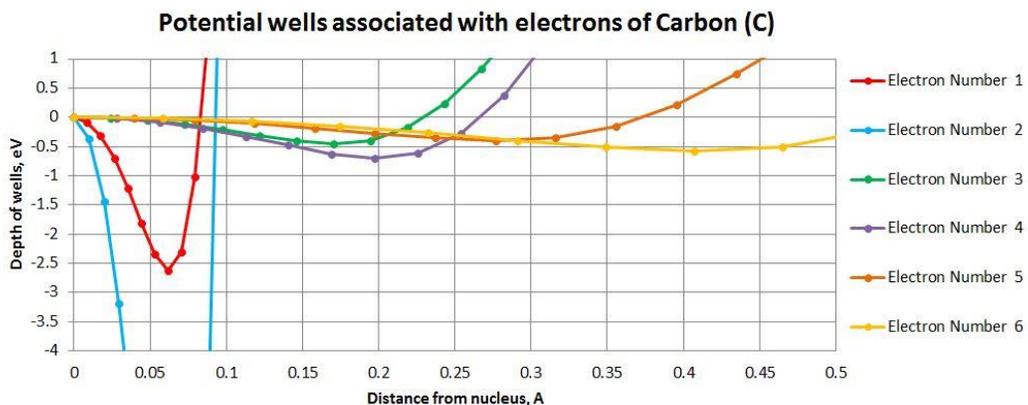


Figure 5: Nuclear potential wells associated with the electrons of Carbon atom

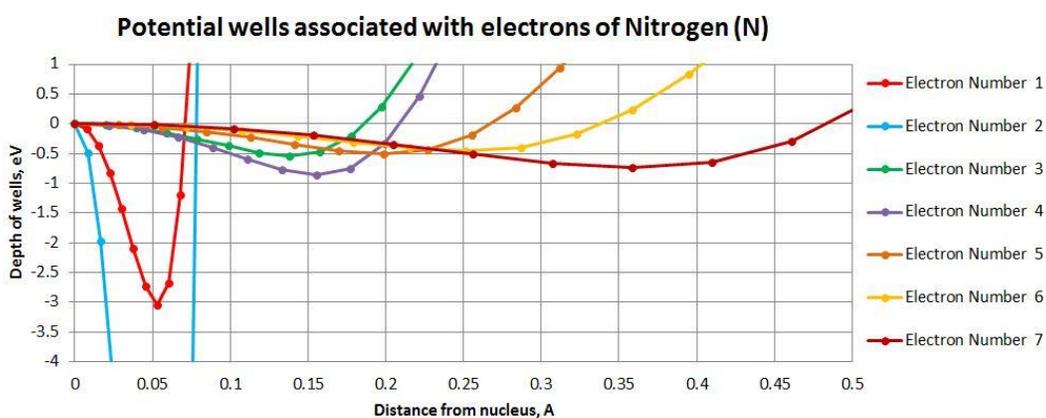


Figure 6: Nuclear potential well associated with the electrons of Nitrogen atom

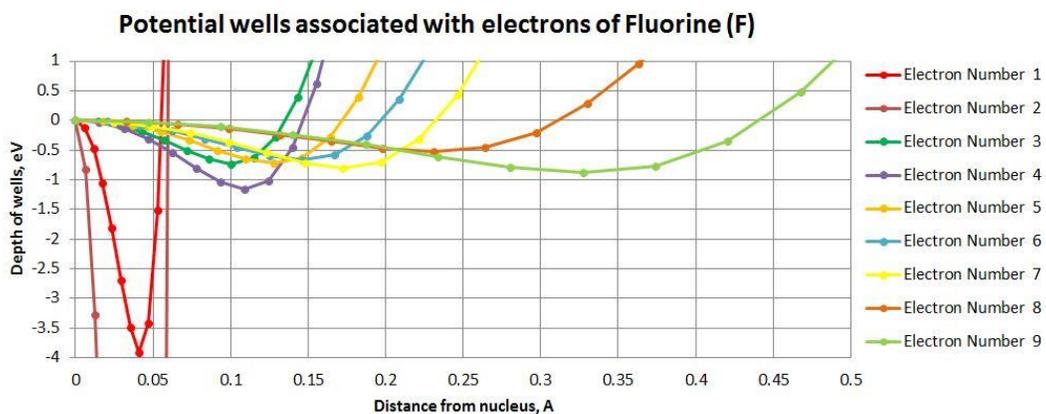


Figure 7: Nuclear potential wells associated with the electrons of Fluorine atom

Element	Atomic Number	Electron Number [#]	App. Nuclear Charge (ANC)	Bohr Orbital Radius, A	Well Distance, A	Well Depth, eV
Hydrogen (H)	1	e1	1.0	0.529	0.370	-0.693
Helium (He)	2	e1	1.344	0.394	0.276	-1.253
		e2	0.656	0.265	0.185	-0.909
Lithium (Li)	3	e1	0.629	0.840	0.588	-0.275
		e2	1.728	0.224	0.157	-2.825
		e3	0.642	0.176	0.123	-1.335
Beryllium (Be)	4	e1	0.827	0.639	0.447	-0.475
		e2	0.328	0.457	0.320	-0.263
		e3	2.206	0.157	0.110	-5.144
		e4	0.636	0.132	0.093	-1.765
Boron (B)	5	e1	0.780	0.678	0.474	-0.422
		e2	0.577	0.389	0.272	-0.544
		e3	0.309	0.317	0.222	-0.357
		e4	2.696	0.121	0.085	-8.161
		e5	0.633	0.106	0.074	-2.196
Carbon (C)	6	e1	0.908	0.582	0.407	-0.573
		e2	0.427	0.395	0.277	-0.396
		e3	0.535	0.282	0.197	-0.696
		e4	0.299	0.243	0.170	-0.452
		e5	3.189	0.099	0.069	-11.872
		e6	0.631	0.088	0.062	-2.626
Nitrogen (N)	7	e1	1.031	0.512	0.358	-0.739
		e2	0.439	0.359	0.251	-0.449
		e3	0.389	0.283	0.198	-0.504
		e4	0.516	0.222	0.155	-0.854
		e5	0.293	0.197	0.138	-0.545
		e6	3.685	0.083	0.058	-16.277
		e7	0.629	0.076	0.053	-3.054
Oxygen (O)	8	e1	0.996	0.529	0.370	-0.691
		e2	0.602	0.329	0.231	-0.671
		e3	0.399	0.263	0.184	-0.555
		e4	0.372	0.222	0.155	-0.615
		e5	0.504	0.183	0.128	-1.011
		e6	0.289	0.166	0.116	-0.638
		e7	4.182	0.072	0.050	-21.375
		e8	0.627	0.066	0.046	-3.482
Fluorine (F)	9	e1	1.126	0.468	0.327	-0.884
		e2	0.466	0.330	0.231	-0.518
		e3	0.538	0.246	0.173	-0.801
		e4	0.379	0.209	0.146	-0.665
		e5	0.361	0.183	0.128	-0.725
		e6	0.495	0.156	0.109	-1.167
		e7	0.285	0.143	0.100	-0.729
		e8	4.679	0.063	0.044	-27.166
		e9	0.626	0.059	0.041	-3.906

e1 refers to the electron which is furthest away from nucleus.

Table 1: Numerical data related to nuclear potential wells of atoms

Figures 5, 6, and 7 present the wells associated with electrons of Carbon, Nitrogen, and Fluorine. As one may observe, the first two wells corresponding to the s shell electrons of

these atoms are also closer to their nuclei and those wells are quite deep. But with respect to other valance electrons, the wells are further away from nuclei and are shallow.

Table 1 presents the same subject but through numerical data. The name of atoms, atomic numbers, ANC, Bohr orbital radii, well distance from nuclei, and depth of wells in eV are listed in the table for all electrons of each atom.

A new outlook for the atomic internal structure:

The concept of nuclear potential wells in vicinity of nuclei and the settlement of electrons with their center of gravities at their corresponding wells portrays a different view of atoms and the related chemical bonds. Figure 8 provides a graphical presentation of the case considering those concepts. The sketch on the left side of the figure presents an atom with just one electron (i.e. Hydrogen) with its center of gravity at its own well. The right side sketch of the figure shows an atom with two electrons (i.e. Helium) with the center of gravity of electrons residing at their wells and on the opposite sides of nucleus. Hydrogen with one electron (unpaired) is chemically active, while Helium with two electrons (a paired set) is fully covered and chemically inactive. Hydrogen and Helium atoms have low atomic numbers and therefore they cannot accommodate more electrons.

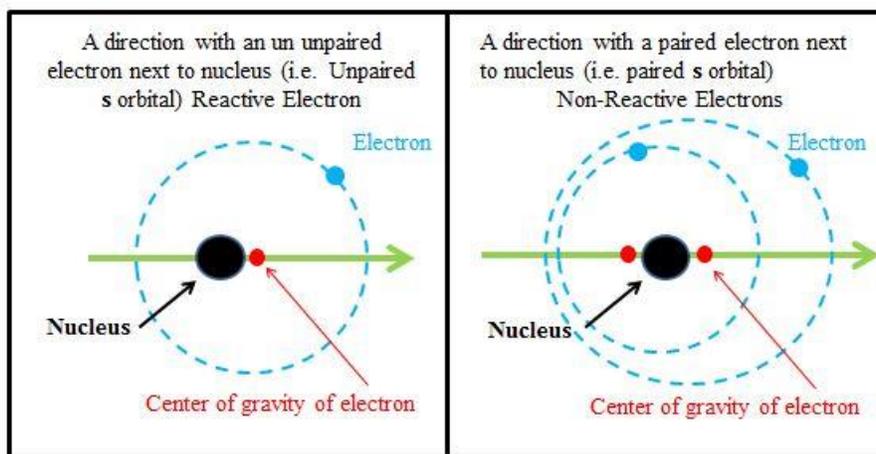


Figure 8: Location of center of gravity of electrons with respect to nucleus for reactive and non-reactive electrons in a direction (i.e. s orbital)

Meanwhile other atoms with higher number of atomic numbers can accommodate more electrons such as (sp) shell with 8 electrons, (d) shell with 10 electrons and (f) shell with 14 electrons as discussed in earlier publications [1-3]. Then the next question would be about the arrangement and organization of electrons in those shells which contain larger numbers of electrons. Figure 9, 10, and 11 provide rough views of the (sp), (d), and (f) electronic shells.

Figure 9 portrays the (sp) shell with 8 electrons. As one can imagine, the only reasonable shape of the shell would be a tetrahedron with 4 faces and 4 vertices in 4 different directions. In a symmetrical case, tetrahedron would have six 109.471 degree angles between 4 different directions as shown in the Figure 9. A completed (sp) shell would

have four pairs of electron in 4 different directions. Atoms would be inactive in the directions with two electrons (paired) and active in the directions with only one electron. A paired electron in a direction would cover the nucleus from both sides and would not allow the atom to react in that direction.

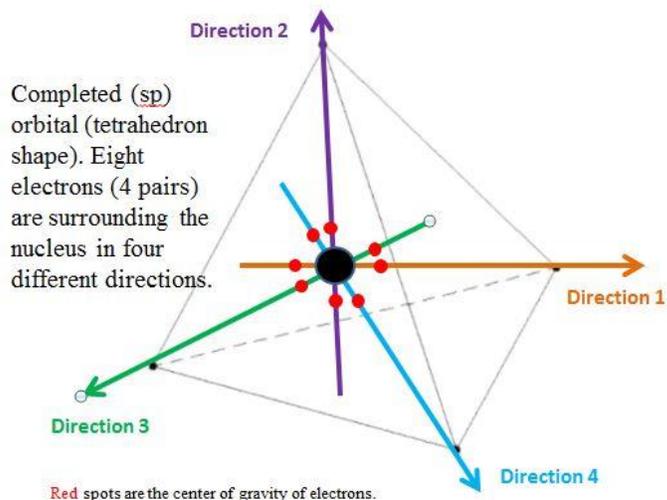


Figure 9: Completed (sp) orbital with 8 paired electrons in 4 directions.

Figure 10 portrays the (d) shell with 10 electrons. As one can imagine, a reasonable shape of the shell would be a pentahedron with 5 faces and 5 vertices in 5 different directions. A pentahedron may have six 120 and four 75.522 degree angles (total of 10 angles) between 5 different directions as shown in the figure. A completed (d) shell would have five pairs of electrons in 5 different directions. Again atoms with (d) orbital would be inactive in the directions with two electrons (paired) and active in the directions with only one electron. A paired electron in a direction would cover the nucleus from both sides and would not allow the atom to react in that direction.

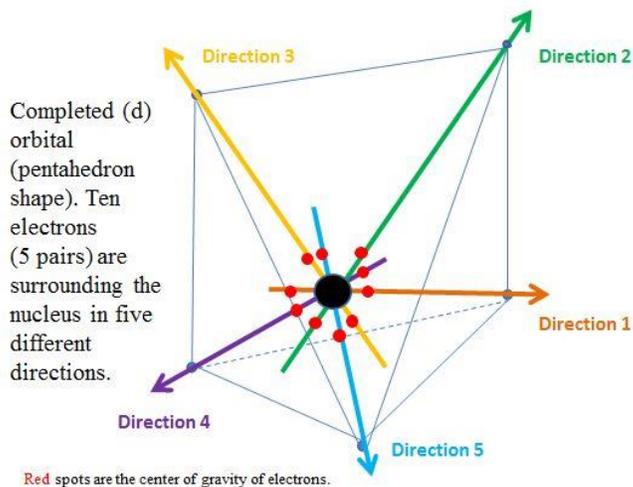


Figure 10: Completed d orbital with 10 paired electrons in 5 directions.

Figure 11 portrays the (f) shell with 14 electrons. As one can imagine, a reasonable shape of the shell would be a heptahedron with 7 faces and 7 vertices in 7 different directions. A heptahedron may have three 120, five 60, six 97.181 and six 128.682 degree angles (total of 20 angles) between 7 different directions as shown in the figure. A completed (f) shell would have seven pairs of electrons in 7 different directions. Again atoms with (f) orbital would be inactive in the directions with two electrons (paired) and active in the directions with only one electron. A paired electron in a direction would cover the nucleus from both sides and would not allow the atom to react in that direction.

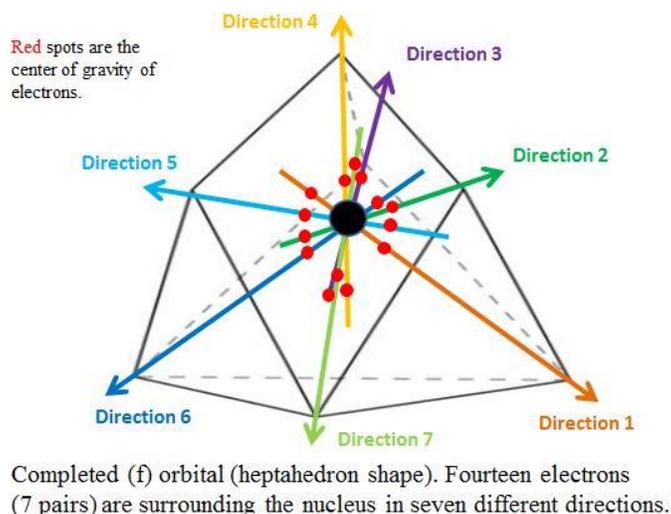


Figure 11: Completed f orbital with 14 paired electrons in 7 directions.

What we can learn from Hydrogen molecule:

Next is imperative to look at the Hydrogen molecule to better understand the mechanism of a chemical bond. The Hydrogen atom is small and probably does not have a size constraint in reactions. The experimental figure for the bond length of Hydrogen molecule is 0.74 Å. Meanwhile, the calculated radius of Bohr atomic model for Hydrogen atom is 0.52924 Å with a well distance of 0.370468 Å. The well distance is the distance between the center of gravity of electron in the well and the nucleus which is exactly 70% of the related Bohr atomic orbital radius. Those figures show that the bond length of Hydrogen molecule is exactly twice of the related well distance (i.e. $0.74 = 2 \times 0.37$). This means that if the two reacting atoms are sufficiently small and there is no size constraint for the two to get close, the two atoms involved in the chemical bond would get close enough to each other to overlap the center of gravity of their electrons. But atoms with larger sizes show longer bond lengths than summation of well distances due to their higher atomic numbers and sizes. Therefore, one may make a conclusion that the bond lengths are dependent on the well distances and also atomic numbers of atoms involved in the reaction (Eq. 18).

$$\text{Bond Lengths} = f(\text{well distances, atomic numbers}) \quad (18)$$

It should be noted that there might be other parameters affecting the bond lengths which is not known to the author.

Summary of Approach:

Hence the suggested methodology in this article utilizes the following concepts and steps:

- Bohr one-electron atomic model is used for calculation of orbital radii.
- Chemical bonds are treated as bonds between two one-electron atoms.
- Multi-electron atoms are converted to one-electron atoms by grounding inactive non-reacting electrons onto their nuclei.
- The concepts of Apparent Nuclear Charge (ANC) and Electron Shielding Effect (ESE) explained in previous literatures [1-3] are utilized to ground inactive electrons.
- The distance of nuclear potential wells from the corresponding nuclei for the participating electrons in the bond(s) are computed and utilized.
- The sizes of participating atoms in the bond are taken into account by utilizing their atomic numbers.
- Bond indices (BI's) are defined for single, double and triple bonds using the distances of nuclei from the potential wells of the reacting electrons (i.e. WD₂₃ means well distance of electron number 3 of the atom number 2) and atomic numbers (i.e. AN₂ means atomic number of atom number 2) of reacting atoms.
- Bond Indices (BI) are defined according to the following formulas:

$$\begin{aligned} \text{BI (single bonds)} &= (\text{AN}_1.\text{AN}_2)^{0.5} . (\text{WD}_{11}.\text{WD}_{21})^1 \\ \text{BI (double bonds)} &= (\text{AN}_1.\text{AN}_2)^{0.5} . (\text{WD}_{11}.\text{WD}_{12}.\text{WD}_{21}.\text{WD}_{22})^{0.471} \\ \text{BI (triple bonds)} &= (\text{AN}_1.\text{AN}_2)^{0.5} . (\text{WD}_{11}.\text{WD}_{12}.\text{WD}_{13}.\text{WD}_{21}.\text{WD}_{22}.\text{WD}_{23})^{0.297} \end{aligned}$$

- The definition of bond index (BI) and accuracy of results might be improved by introducing more factors into the bond index as well as using more accurate experimental data. The defined bond index for single bonds is only for the first and outmost electrons. Inner valance electrons if being used in calculations probably need a different parametrization.
- A characteristic curve is fitted onto the experimental data versus bond index.
- The characteristic curve/formula obtained in the previous step is later used to find the unknown bond lengths.

Figure 12 present the pattern of about 90 experimental bond lengths [35-38] versus their defined Bond Indices (BI). The graph shows that the defined BI is actually effective to sort out the experimental bond lengths in harmony and in an order that a characteristic curve could be fitted onto the data. The type and degree of the fitted curves depends on the type of application but the author did not want to exceed more than a third degree polynomial for the fitted curves. With the use of more accurate experimental data and investigation of other possible parameters affecting the bond lengths, there might be a possibility to further develop the methodology and increase the accuracy of the approach.

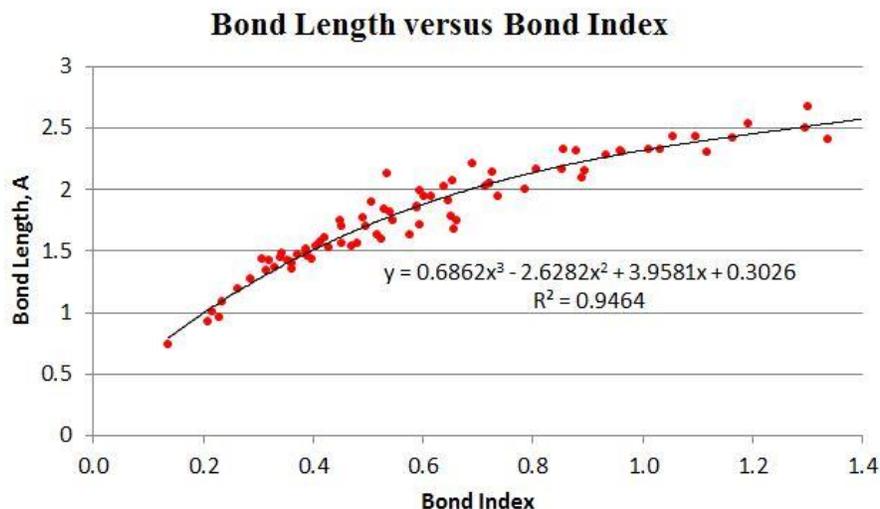


Figure 12: Fitted curve on experimental data of bond lengths

Table 2: Calculated single, double, and triple bonds using the presented method in this article and the corresponding errors

Single Bonds						
	Molecule	Model 1 Calc. Bond Length, Å	Model 2 Calc. Bond Length, Å	Experimental* Bond Length, Å	Model 1 Error, %	Model 2 Error, %
1	C-C	1.52227	1.50549	1.54	1.2%	2.2%
2	N-N	1.37088	1.3741	1.45	5.5%	5.2%
3	O-O	1.48195	1.4698	1.48	0.1%	0.7%
4	F-F	1.32593	1.33637	1.42	6.6%	5.9%
5	Si-Si	2.19599	2.20846	2.33	5.8%	5.2%
6	P-P	2.00688	1.98623	2.21	9.2%	10.1%
7	S-S	2.04683	2.03129	2.05	0.2%	0.9%
8	Cl-Cl	1.86928	1.83825	1.99	6.1%	7.6%
9	Ge-Ge	2.53619	2.59117	2.41	5.2%	7.5%
10	As-As	2.38657	2.44593	2.43	1.8%	0.7%
11	Br-Br	2.26636	2.29631	2.28	0.6%	0.7%
12	I-I	2.51408	2.57533	2.67	5.8%	3.5%
				Overall Avg Error =	4.6%	4.8%
Double Bonds						
	Molecule	Model 1 Calc. Bond Length, Å	Model 2 Calc. Bond Length, Å	Experimental* Bond Length, Å	Model 1 Error, %	Model 2 Error, %
1	C=C	1.3054	1.29408	1.34	2.6%	3.4%
2	C=N	1.25339	1.25143	1.29	2.8%	3.0%
3	C=O	1.25982	1.25623	1.20	5.0%	4.7%
4	C=S	1.5359	1.48742	1.60	4.0%	7.0%
5	N=N	1.20324	1.21104	1.25	3.7%	3.1%
6	N=O	1.20944	1.21558	1.21	0.0%	0.5%

7	P=O	1.50196	1.45661	1.50	0.1%	2.9%
8	P=S	1.80533	1.73826	1.86	2.9%	6.5%
9	O=O	1.21567	1.22014	1.21	0.5%	0.8%
10	S=O	1.48452	1.44113	1.43	3.8%	0.8%
11	S=S	1.78666	1.71929	1.49	19.9%	15.4%
12	Se=Se	2.19154	2.16537	2.15	1.9%	0.7%
				Average Error =	3.9%	4.1%
Triple Bonds						
	Molecule	Calc. model 1 Bond Length, A	Calc. model 2 Bond Length, A	Experimental* Bond Length, A	Model 1 Error, %	Model 2 Error, %
1	C≡C	1.15349	1.1634	1.20	3.9%	3.1%
2	C≡N	1.13484	1.14849	1.16	2.2%	1.0%
3	C≡O	1.13201	1.14585	1.13	0.2%	1.4%
4	N≡N	1.1165	1.13393	1.10	1.5%	3.1%
				Average Error =	1.9%	2.1%

*- Experimental data [35-38]

Results:

Numerical results for tens of single, double, and triple bonds are presented in Table 2 and the attachment 1. The overall average error for all calculated bond lengths in this table and attachment 1 was less than 5%. Single bonds showed an overall error of 4.6 to 4.8% while double bonds had about 3.9 to 4.1% error and triple bonds showed 1.9 to 2.1% error. The overall average accuracy for the computed bonds is above 95% which might be encouraging for those who may want to continue this line of work. The error might be due to quality of parameterization as well as other unknown factors.

Software:

This article accompanies a computer software program that might be helpful to readers to find or estimate an unknown chemical bond length using the methodology outlined in this article. The software is only for research and educational purpose and not for commercial use. The software can be used for all elements in the periodic table with atomic numbers up to 108 without a need for any additional tools. Attachment 2 of the article provides more information in this regard.

Conclusion:

Earlier atomic and molecular theories were briefly reviewed. The new concept of converting multi-electron reactants to one-electron atoms by grounding the inactive non-reacting electrons of the reactants using the ANC and ESE concepts discussed in previous literature was described and utilized. The nuclear potential wells were introduced with several examples for different atoms using the related numerical values and graphs. Bohr one-electron atomic model together with the related nuclear wells were utilized to obtain the related bond lengths. A different concept to explain the active and inactive electrons in chemical reactions was discussed and explained with the help of a few graphs. The new approach was tested and the accuracy was reported. A computer software program to

calculate bond lengths between the elements of periodic table was developed and submitted for the use of readers. The average error by using this methodology was found to be less than 5% for about ninety chemical bonds.

Author Declaration:

1. Funding (information that explains whether and by whom the research was supported)
[There was no funding for this research work.](#)
2. Conflicts of interest/Competing interests (include appropriate disclosures)
[There is no conflict of interest for this research work.](#)
3. Availability of data and material (data transparency)
[All data and material were submitted with full transparency.](#)
4. Code availability (software application or custom code)
[A computer software program was prepared for readers which will be submitted upon receiving guidelines with respect to the email address for submittal.](#)
5. Authors' contributions (include appropriate statements)
[There is only one author who contributed all of the research work.](#)

References:

1. Zadeh DH, (2019) A new approach to estimate atomic energies, J Mol Model 25, 366 <https://doi.org/10.1007/s00894-019-4259-1>
2. Zadeh DH, (2019) Atomic shells according to ionization energies, J Mol Model 25 (8), 251 <https://link.springer.com/article/10.1007/s00894-019-4112-6>
3. Zadeh DH, (2017) Electronic structures of elements according to ionization energies, J Mol Model 23(12),357 <https://link.springer.com/article/10.1007/s00894-017-3534-2>
4. Murray JS, Zadeh DH, Lane P, Politzer P (2018) The role of ‘Excluded’ electronic charge in noncovalent interactions, Molecular Physics, <https://www.tandfonline.com/doi/abs/10.1080/00268976.2018.1527044>
5. Zadeh DH, Murray JS, Redfern PC, Politzer P (1991) Computational study of the nitrogen-nitro rotational energy barriers in some aliphatic and alicyclic nitramines , J Phys Chem 95(20):7702–7709, <https://doi.org/10.1021/j100173a028>
6. Zadeh DH, Grodzicki M, Seminario JM, Politzer P (1991) Computational study of the concerted gas-phase triple dissociations of 1, 3, 5-triazacyclohexane and its 1, 3, 5-trinitro derivative (RDX), J Phys Chem 95:7699, <https://doi.org/10.1021/j100173a027>
7. Zadeh DH, Murray JS, Grodzicki M, Seminario JM, Politzer P (1992) C-H Bond dissociation of acetylene: Local density functional calculations, Int J Quantum Chem 42:267–272, <https://doi.org/10.1002/qua.560420203>
8. Zadeh DH, Murray JS, Grice ME, Politzer P (1993) X–NO₂ rotational energy barriers: Local density functional calculations, Int J Quantum Chem 45:15–20, <https://doi.org/10.1002/qua.560450104>
9. Politzer P, Zadeh DH (1993) Relationship between dissociation energies, force constants, and bond lengths for some N–F and O–F bonds, J Chem Phys 98(9):7659, <https://doi.org/10.1063/1.464679>
10. Politzer P, Zadeh DH (1994) Bond-Breaking Energies for 2, 2'-Dichlorodiethyl Sulfide (Sulfur Mustard) in Media of Different Dielectric Constants, J Phys Chem 98:1576–1578, <https://doi.org/10.1021/j100057a008>
11. Grice ME, Zadeh DH, Politzer P(1994) Calculated structure, heat of formation and decomposition energetics of 1, 3-dinitro-1, 3-diazacyclobutane, J Chem Phys 100 (6): 4706–4707, <https://doi.org/10.1063/1.466257>
12. Zadeh DH, Grice ME, Concha MC, Murray JS, Politzer P (1995) Nonlocal density functional calculation of gas phase heats of formation, J Comput Chem 16(5):654–

- 658, <https://doi.org/10.1002/jcc.540160513>
13. Politzer P, Concha MC, Grice ME, Murray JS, Lane P, Zadeh DH (1998) Computational investigation of the structures and relative stabilities of amino/nitro derivatives of ethylene, *J Mol Struct (THEOCHEM)* 452:75–83; https://homepage.univie.ac.at/mario.barbatti/papers/nitroethylene/politzer_theochem_1998.pdf
 14. Bohr N (1913) The Spectra of Helium and Hydrogen, *Nature* 92: 231–232; <https://doi.org/10.1038/092231d0>
 15. Bohr N (1913) On the Constitution of Atoms and Molecules, Part I, *Phil Mag* 26 (151): 1–24; <https://doi.org/10.1080/14786441308634955>
 16. Hehre WJ, Radom L, Schleyer PVR, Pople JA (1986) *Ab initio molecular orbital theory*. Wiley, New York; <https://doi.org/10.1002/jcc.540070314>
 17. Sharpe AG (1986) *Inorganic chemistry*. Longman, London and New York; <https://doi.org/10.1002/bbpc.19860901144>
 18. Szabo A, Ostlund NS (1989) *Modern quantum chemistry*. McGraw-Hill, New York, ISBN-10: 0486691861
 19. Atkins PW (1986) *Physical Chemistry*, W.H. Freeman and Company, New York, ISBN-10: 0716731681
 20. Drago RS (1977) *Physical Methods in Chemistry*. Saunders College Publishing, Philadelphia, ISBN-10: 0721631843
 21. Pauling L, Wilson EB (1985) *Introduction to Quantum Mechanics with Applications to Chemistry*. Dover Publications, INC., New York, ISBN-10:0486648710
 22. Herzberg G (1945) *Atomic Spectra and Atomic Structure*. Dover Publications, New York, ISBN-10:0486601153
 23. Johnson CS, Pedersen LG (1986) *Problems and Solutions in Quantum Chemistry and Physics*. Dover Publications, Inc., New York, ISBN-10:0486151530
 24. Schrödinger, E. (1926) An Undulatory Theory of the Mechanics of Atoms and Molecules, *Physical Review*. **28** (6): 1049–1070; <https://doi.org/10.1103/PhysRev.28.1049>
 25. Hartree, D. R. (1928). "The Wave Mechanics of an Atom with a Non-Coulomb Central Field, *Math. Proc. Camb. Philos. Soc.* **24** (1): 111. [doi:10.1017/S0305004100011920](https://doi.org/10.1017/S0305004100011920).
 26. Hartree, D. R.; Hartree, W. (1935) Self-consistent field, with exchange, for beryllium, *Proc. Royal Soc. London, A.* **150** (869), 9; [doi:10.1098/rspa.1935.0085](https://doi.org/10.1098/rspa.1935.0085).
 27. Slater, J. C. (1928). The Self Consistent Field and the Structure of Atoms, *Phys. Rev.* **32** (3): 339–348, [doi:10.1103/PhysRev.32.339](https://doi.org/10.1103/PhysRev.32.339).
 28. Gaunt, J. A. (1928). "A Theory of Hartree's Atomic Fields, *Math. Proc. Camb. Philos. Soc.* **24** (2): 328–342, [doi:10.1017/S0305004100015851](https://doi.org/10.1017/S0305004100015851)
 29. Slater, J. C. (1930). Note on Hartree's Method. *Phys. Rev.* **35** (2): 210–211, [doi:10.1103/PhysRev.35.210.2](https://doi.org/10.1103/PhysRev.35.210.2)
 30. Moller C, Plesset MS (1934) Note on an approximation treatment for many-electron systems, *Phys Rev*, 46, 618; <https://doi.org/10.1103/PhysRev.46.618>
 31. Feynman RP (1939) Forces in molecules, *Phys Rev* 56:340; <https://doi.org/10.1103/PhysRev.56.340>
 32. Hohenberg P, Kohn W (1964) Inhomogeneous electron gas, *Phys Rev B* 136:864; <https://doi.org/10.1103/PhysRev.136.B864>
 33. March NH (1982) Electron density theory of atoms and molecules, *J Phys Chem* 86:2262; <https://doi.org/10.1021/j100209a022>
 34. Milne EA (1927) The total energy of binding of a heavy atom, *Proc Camb Philos Soc* 23:794; <https://doi.org/10.1017/S0305004100015589>
 35. Lide DR (2007) *CRC Handbook of Chemistry and Physics*, CRC Press LLC, Boca Raton, FL ISBN: 0849304881, ISBN13: 9780849304880
 36. Olmsted JA, Williams GM (2011) *Chemistry*, 5th Edition. Wiley, New York ISBN-13: 978-0471478119, ISBN-10: 0471478113
 37. Huheey JE, Keiter EA, Keiter RL (1993) *Inorganic Chemistry: Principles of Structure and Reactivity*. HarperCollins College Publishers, New York, ISBN-13: 978-0060429959, ISBN-10: 006042995X
 38. Cottrell TL (1958) *The Strengths of Chemical Bonds*, Butterworths, London <https://doi.org/10.1002/ange.19600721618>

Figures

Application of Bohr Model for the ground state Hydrogen (without the use of DeBroglie's hypothesis)

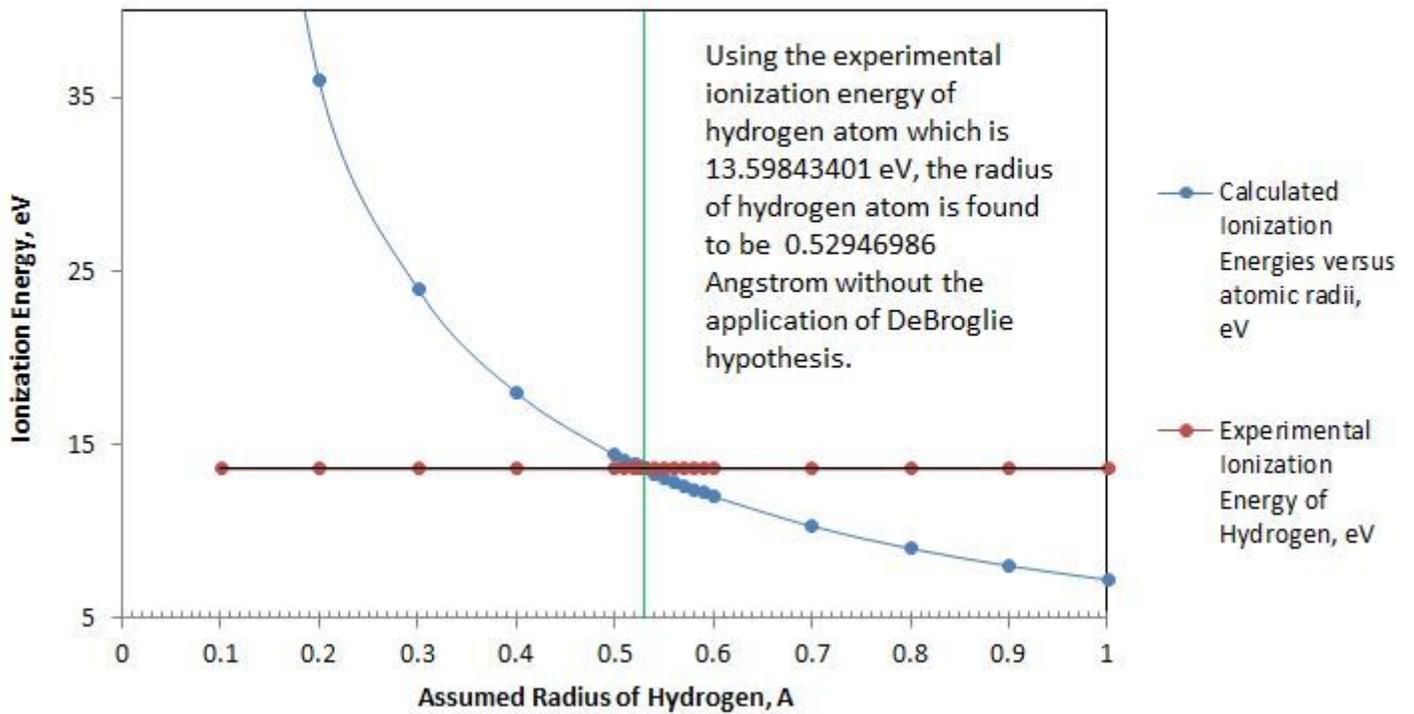


Figure 1

Graphical presentation of the application of Bohr Atomic Model

Potential well associated with the electron of Hydrogen (H)

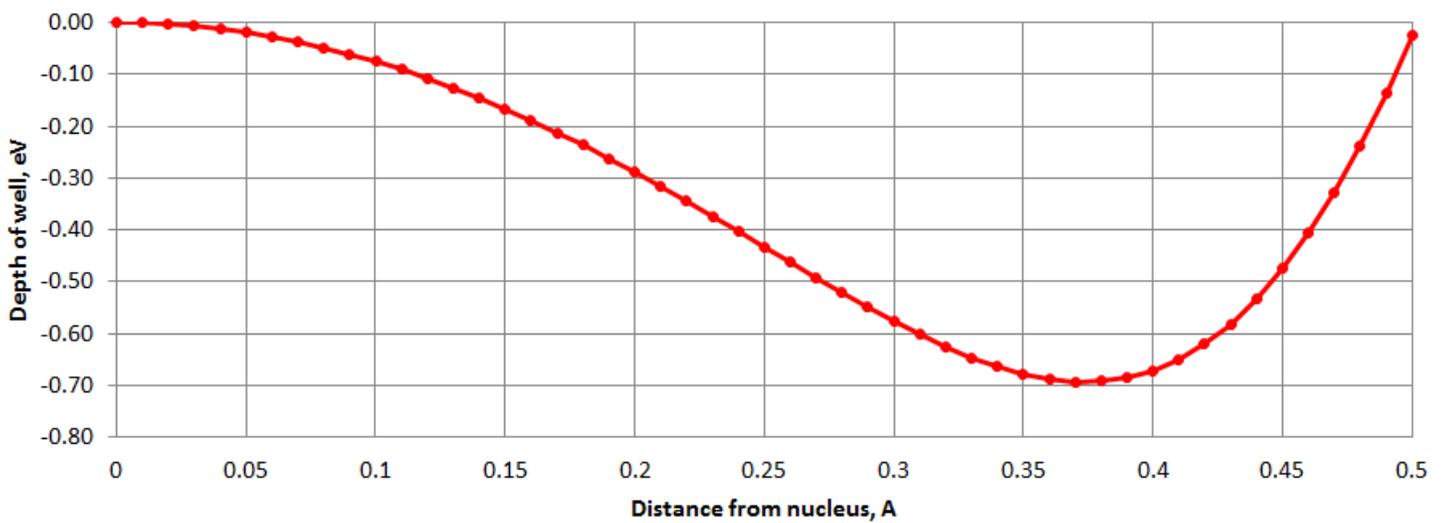


Figure 2

Nuclear potential well associated with the electron of Hydrogen atom

Potential wells associated with electrons of Helium (He)

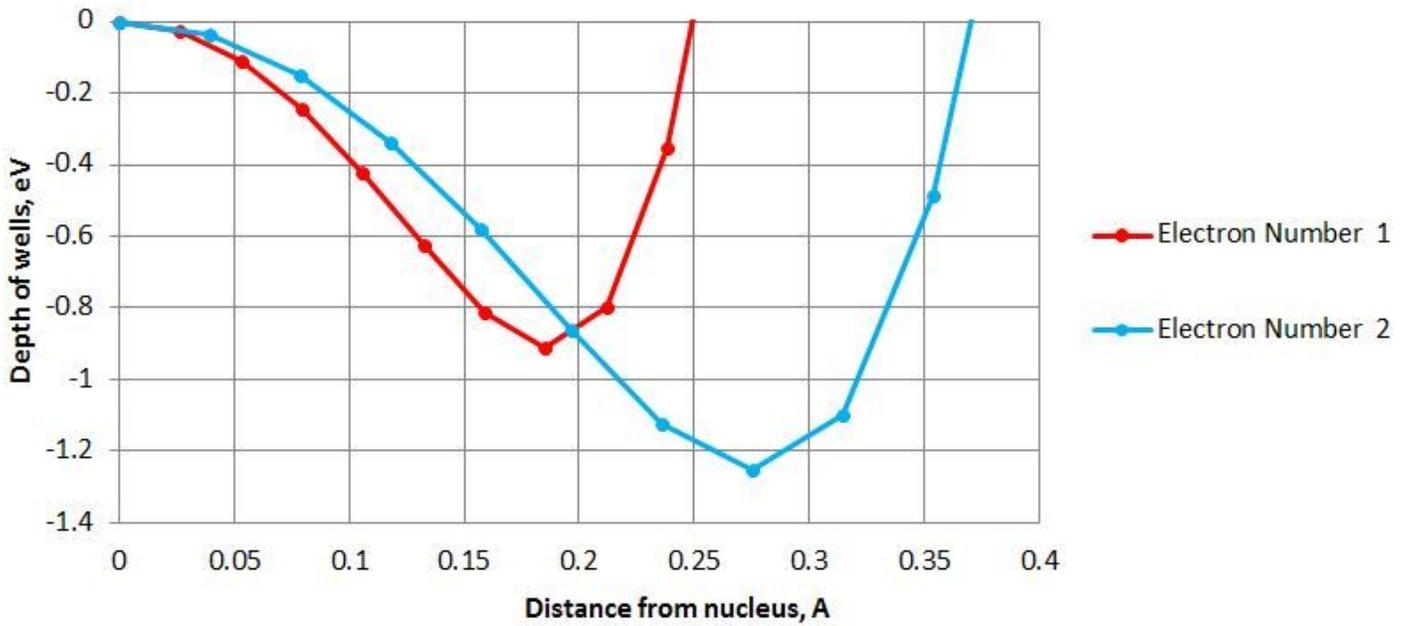


Figure 3

Nuclear potential wells associated with the electrons of Helium atom

Potential wells associated with electrons of Boron (B)

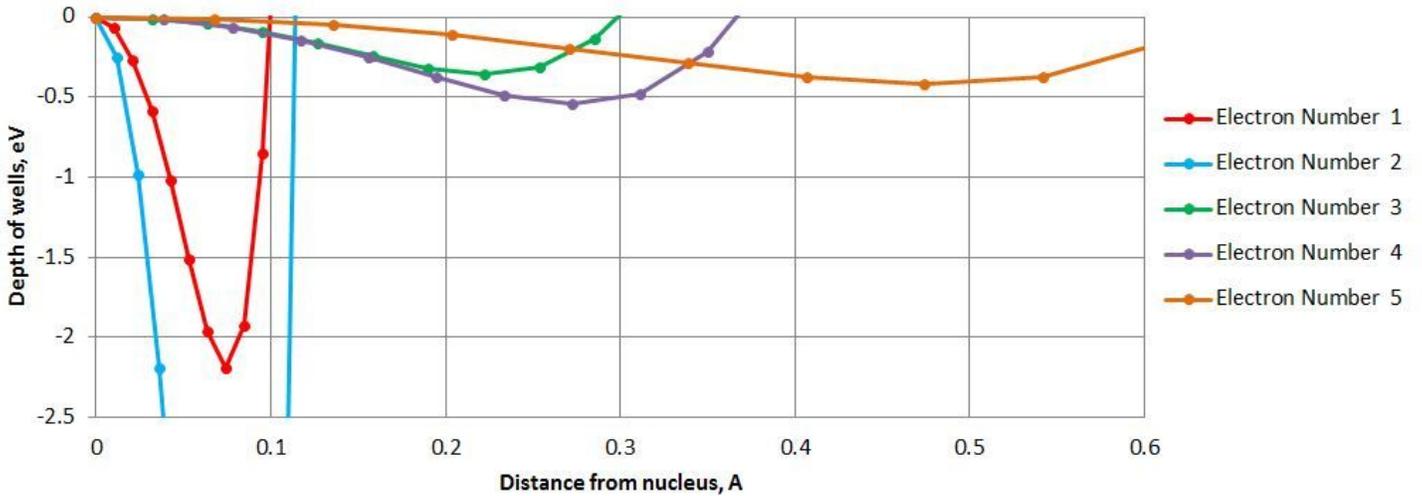


Figure 4

Nuclear potential well associated with the electrons of Boron atom

Potential wells associated with electrons of Carbon (C)

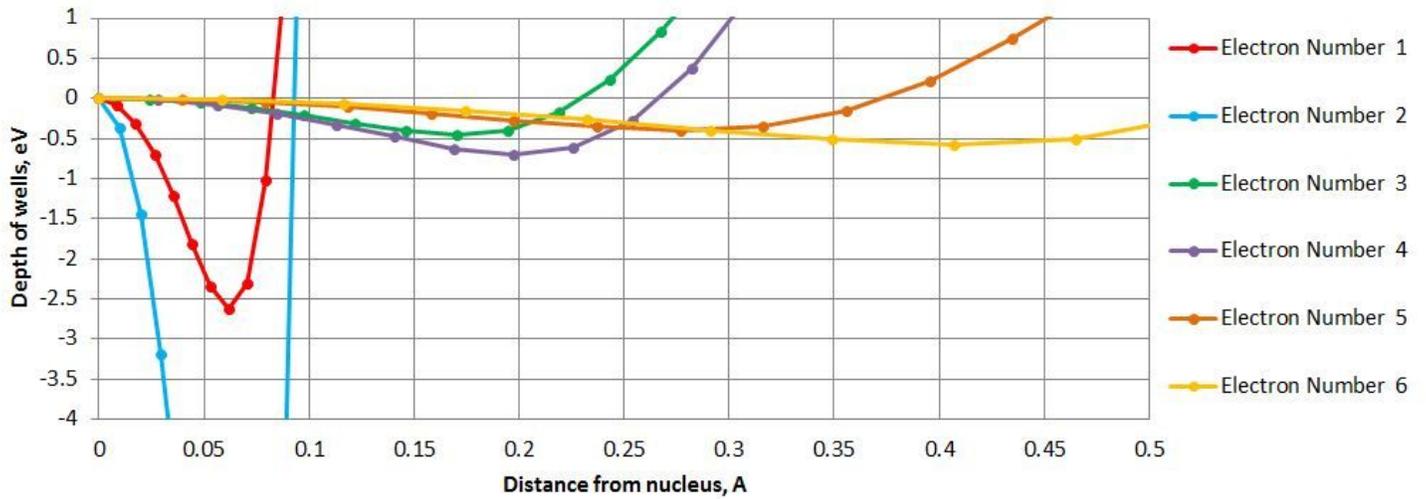


Figure 5

Nuclear potential wells associated with the electrons of Carbon atom

Potential wells associated with electrons of Nitrogen (N)

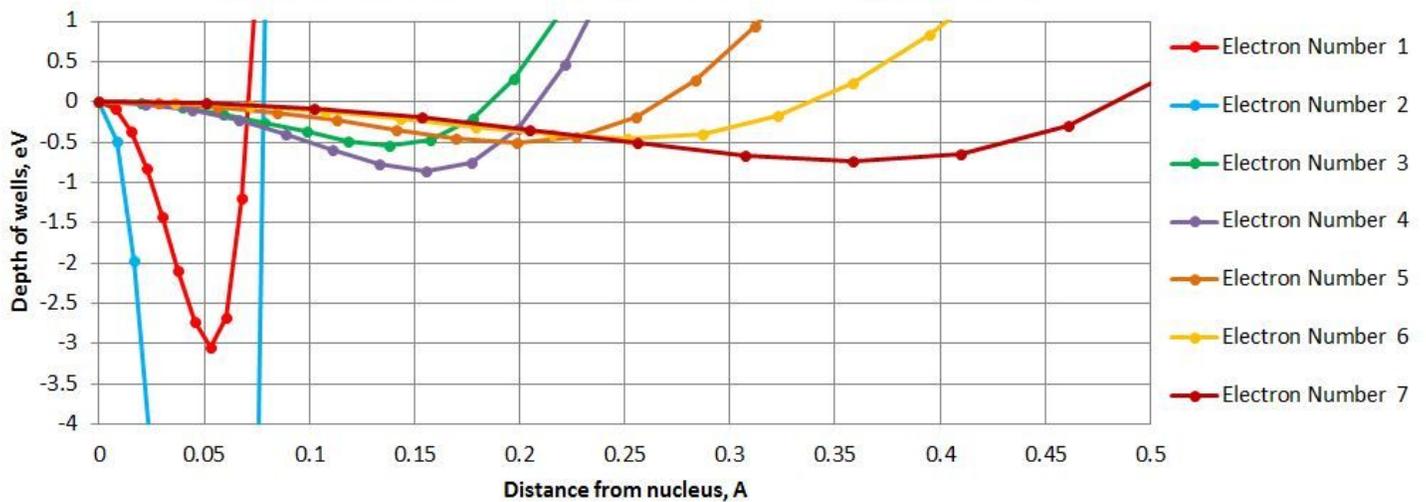


Figure 6

Nuclear potential well associated with the electrons of Nitrogen atom

Potential wells associated with electrons of Fluorine (F)

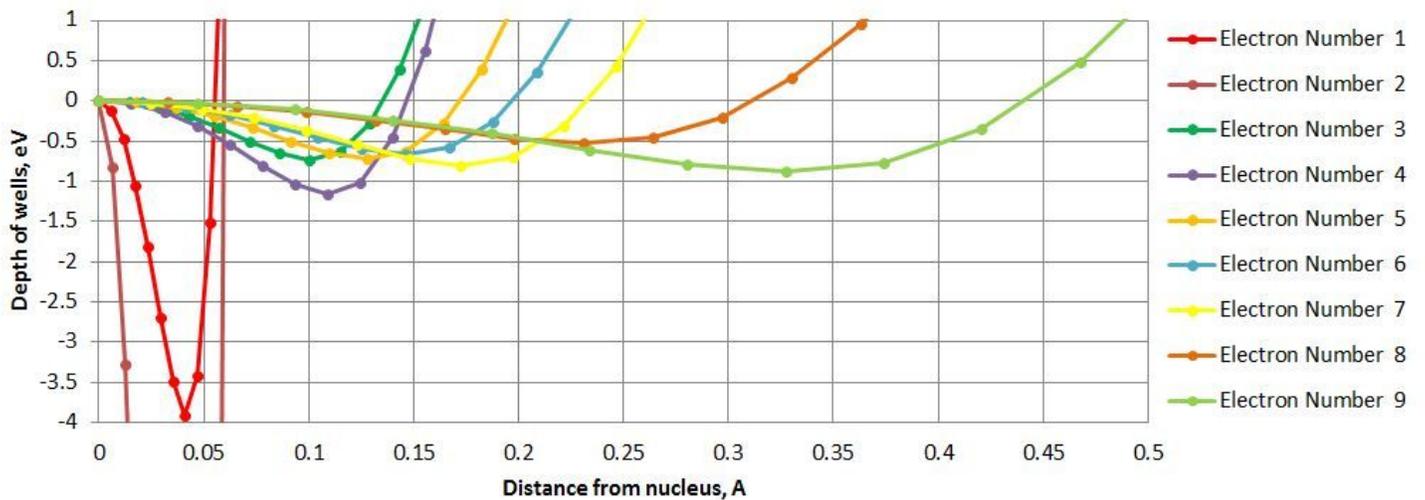


Figure 7

Nuclear potential wells associated with the electrons of Fluorine atom

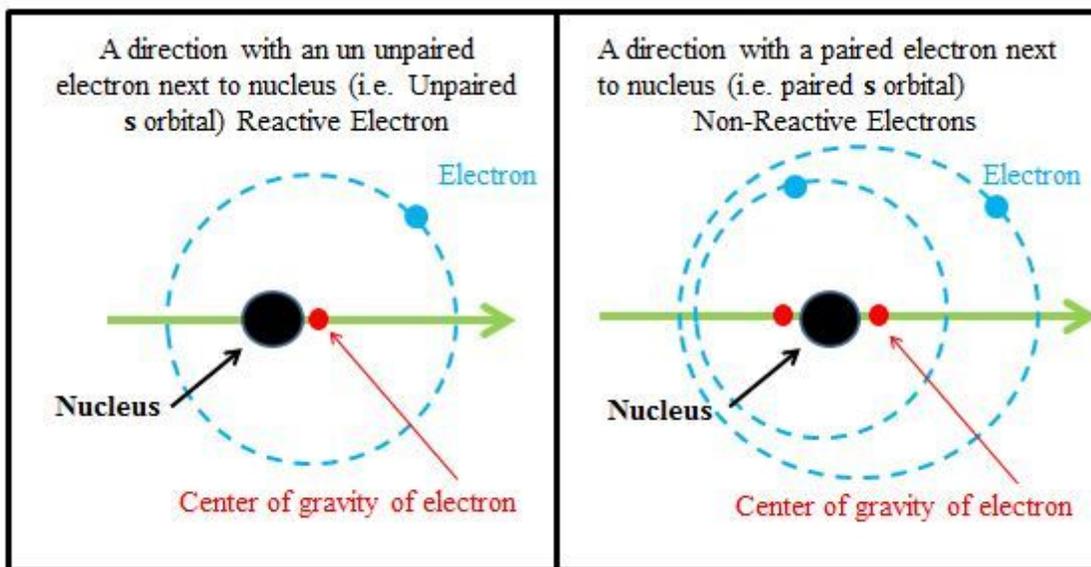


Figure 8

Location of center of gravity of electrons with respect to nucleus for reactive and non-reactive electrons in a direction (i.e. s orbital)

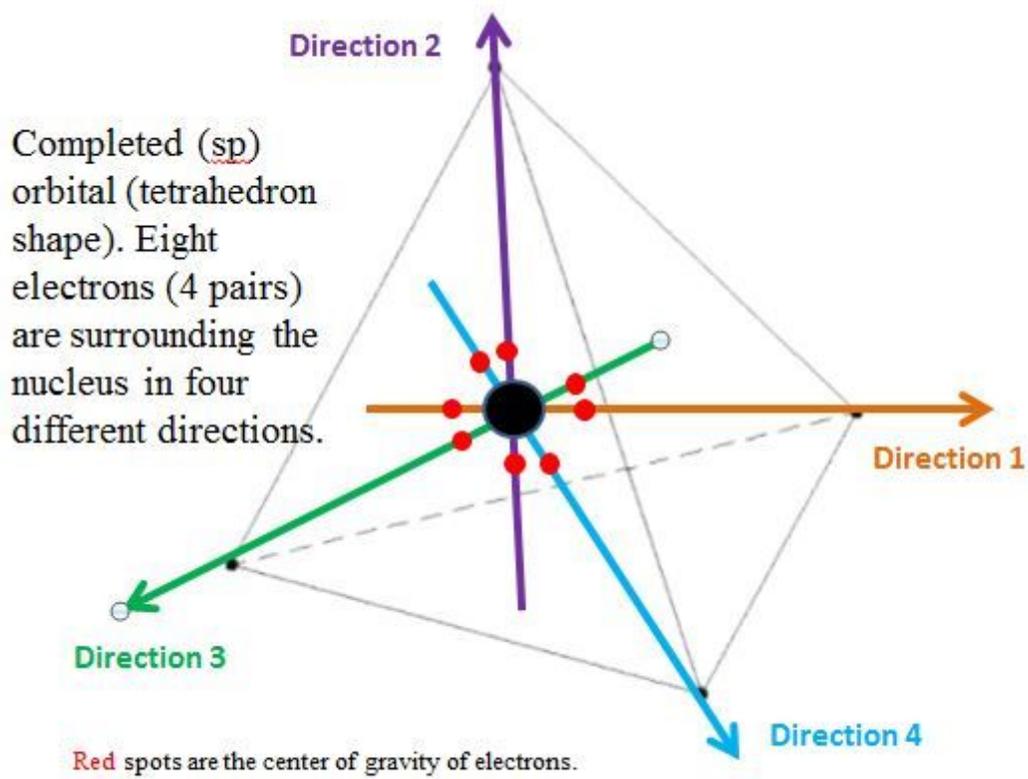


Figure 9

Completed (sp) orbital with 8 paired electrons in 4 directions.

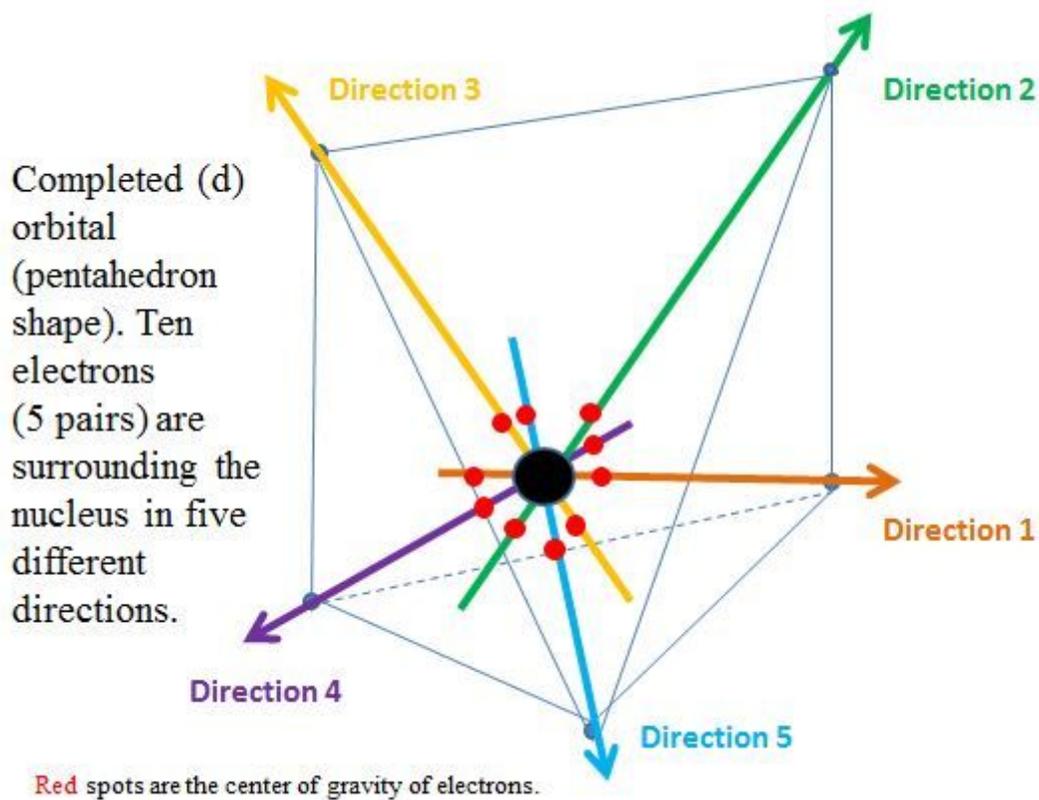
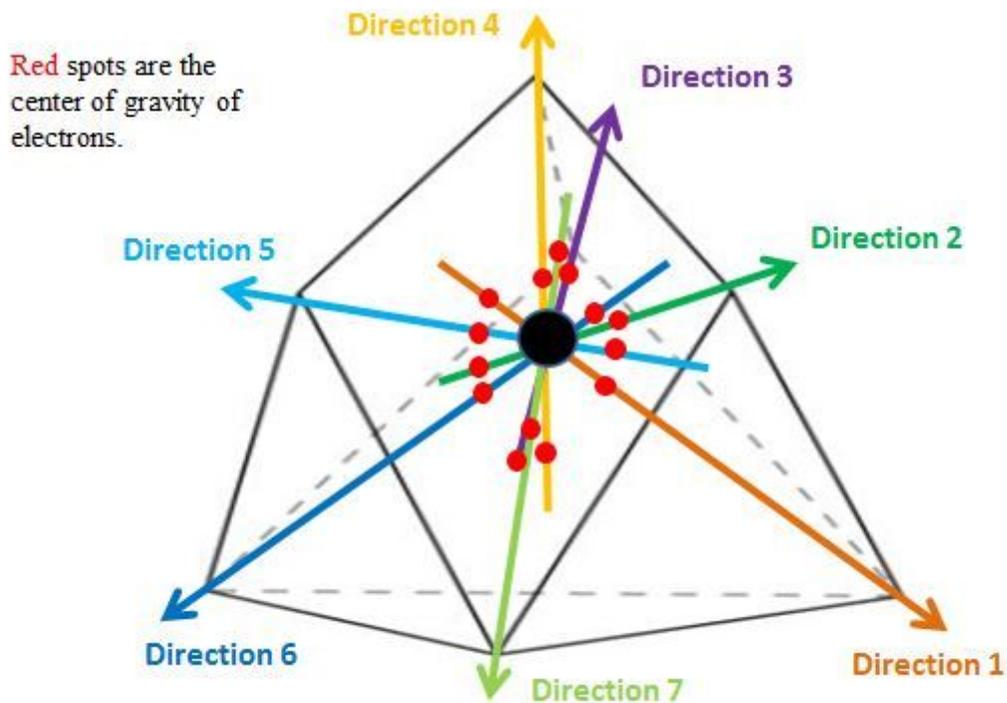


Figure 10

Completed d orbital with 10 paired electrons in 5 directions.



Completed (f) orbital (heptahedron shape). Fourteen electrons (7 pairs) are surrounding the nucleus in seven different directions.

Figure 11

Completed f orbital with 14 paired electrons in 7 directions.

Bond Length versus Bond Index

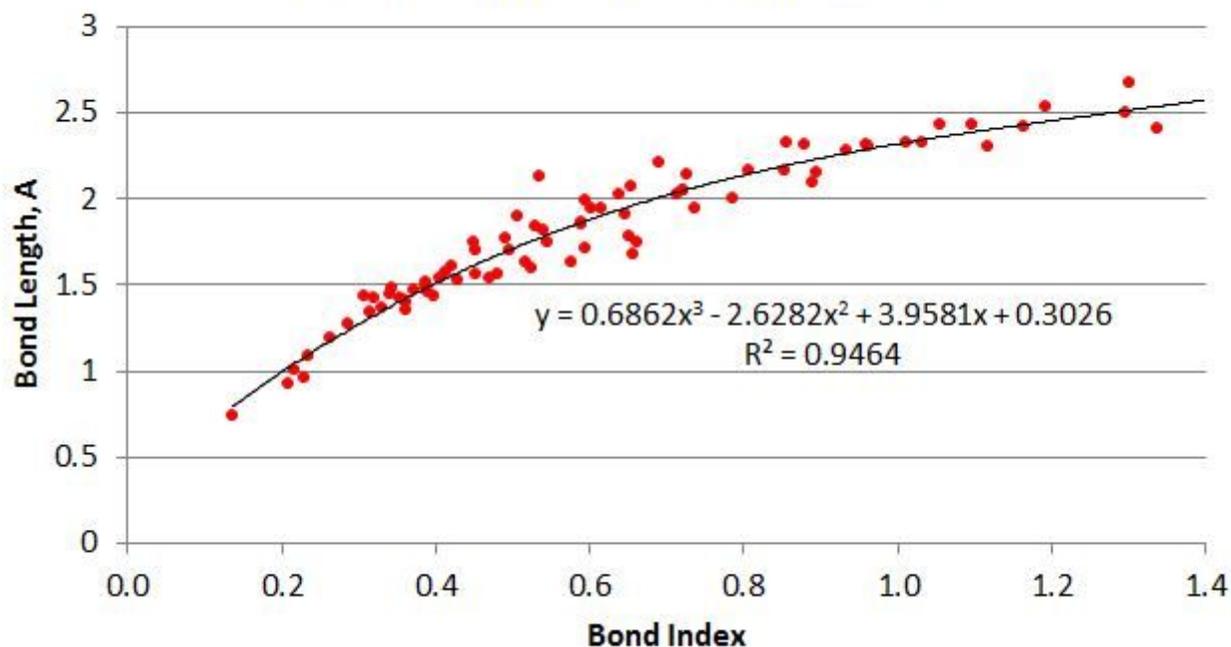


Figure 12

Fitted curve on experimental data of bond lengths

Supplementary Files

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