Evaluation of The Total Attraction Potential of Intra-Shells for Atoms with 5≤Z≤10 Using Hartree-Fock Approximation

Qassim Shamkhi AL-Khafaji   **Kamal Mahdi AL-Harmoosh**

Department of Physics, Faculty of Science University of Kufa.

Qasimsh.alkhfaji@uokufa.edu.iq

Abstract:

This research is used to examine the attraction potential of each intra shells and evaluate the total attraction potential of the atoms using Hartree-Fock approximation and found advantage in contribution ratio of 1s shell and vary in the contribution ratio between 2s and 2p shells.

Keywords: Phthalocyanine, Substrate temperature , Grain size, crystalline, Nano rods.

حساب طاقات الجذب الكلية للأغشية الخارجية في الذرات التي عددها الذري 5≤Z≤10 بأستخدام تقريب هارتري فوك

قاسم شمخي الخفاجي   **كمال مهدي هرموش**

كلية العلوم قسم الفيزياء جامعة الكوفة

الخلاصة:

في هذا البحث تمت دراسة طاقات التجاذب للاغشية الخارجية وحساب طاقة الجذب الكلية للذرات باستخدام تقريب هارتري-فوك وايجاد افضلية نسبة المشاركة في الغلاف 1s والتغاير في نسبة المشاركة بين الغلافين 2s و 2p .

الكلمات المفتاحية: طرق التقريب، الميكانيك الكمي، الفيزياء الذرية، طاقة الجذب.

1. Introduction

Before the quantum mechanics age the scientific look for the wave and particles was like a two separate types of physical entity where the defined wave as a continuous and spatially extended and the particles as discrete with a little or no extension. But the quantum mechanics gives us a new idea for these entities, where the wave sometimes behaves like particle and vise verse. That behavior is called   wave-particle duality.[1] So to describe the wave function of one electron in quantum mechanics we use equation.[2]

$$\phi_{nlm_l m_s} = R_{nl}(r)Y_{ml}(\vartheta,\varphi)\sigma_{m_s}(s)\ldots\ldots(1)$$

Where $\phi_{nlm_l m_s}$ represent the wave function of the electron, $R_n(r)$ the radial function, $Y_{ml}(\vartheta,\varphi)$ the angular function and $\sigma_{m_s}(s)$ is the spin function which takes $\mp\frac{1}{2}$.

Erwin Schrödinger was providing for us his solutions on the wave function to find the eigenvalue of energy and gives us

a good result for atom with only one electron but when the electronic number increases the accuracy to determine energy of the electron decreases. From this point starts the need for the approximation method.

in 1928 when Hartree proposed his theory to calculate the expectation energy of multi-electron atoms by edit on Born-Oppenheimer approximation where he is putting the inter-electron repulsion term in Hamiltonian operator lieu the average repulsion between the electrons ,and used Hartree product to describe the wave-function of system of electrons as in equation.[3]

$$\psi(\chi_1, \chi_2, \ldots, \chi_N) = \phi_1(\chi_1)\phi_2(\chi_2) \ldots \phi_N(\chi_N) \ldots (2)$$

Where ψ is the wave function of multi-electron system, ϕ is the wave function of an electron in the system, χ_i is ith quantum state and N is number of electron in this system.

But Hartree in his theory forgot a very important property of electrons represented by the antisymmetric property.

In 1930 Vladimir Fock assisted Hartree in his theory and providing for us the new method in depending on Slater's determinant to describe the wavefunction of multi-electron atom.[3]

$$\psi(\chi_1, \chi_2, \ldots, \chi_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\chi_1) & \cdots & \phi_1(\chi_N) \\ \vdots & \ddots & \vdots \\ \phi_N(\chi_1) & \cdots & \phi_N(\chi_N) \end{vmatrix} ..(3)$$

2. Theoretical Part

To evaluate the total attraction potential we need to calculate some atomic properties for each intra shells.

In the beginning study the two-electron radial density distribution function $D(r_n, r_m)$ and this property refers to the probability of finding two-electron at distance r_n and r_m simultaneously and it was fund by;[4]

$$D(r_n, r_m) = r_n^2 r_m^2 \int \int \Gamma(x_n, x_m) \, ds_n ds_m d\Omega_n d\Omega_m .(4)$$

Where $\Gamma(r_n, r_m)$ refers to the two electron density function and calculated for each pair of electrons by;[5]

$$\Gamma_{HF}(x_n, x_m) = \frac{1}{2} \sum_{i<j}^{N} B_{ij}^* B_{ij} \ldots \ldots (5)$$

Where $B_{ij} = \phi_i(m)\phi_j(n) - \phi_j(m)\phi_i(n)$

From the two-electron radial density distribution function derivative a very useful property used to calculate the one-electron expectation value and this property is one-electron radial density function $D(r_n)$ and given by; [6]

$$D(r_n) = \int_0^\infty D(r_n, r_m) \, dr_m \ldots \ldots (6)$$

This function is denoted to the probability of finding nth electron at r_n distance.

By using the one electron radial density function in determined the one electron expectation value according to;[7]

$$< r_n^k > = \int_0^\infty D(r_n) r_n^k \, dr_n \ldots \ldots (7)$$

then calculate the standard deviation of one electron expectation value to determine the uncertainty in one particle expectation value;[8]

$$\Delta r_n = \sqrt{< r_n^2 > - < r_n >^2} \ldots \ldots (8)$$

The total attraction potential is equal to summation of the attraction potential of each intra shells and each of them is calculated by a corresponding operator in atomic units;[9]

$$< V_{en} >= \sum_{i=1}^{N} \frac{Z}{<r_i>} \quad \text{...................}(9)$$

3. Results and discussion

In this study we present the results of atomic properties for intra shells of some atoms in the ground state   (B, C, N, O, F and Ne), where each atom contains three intra shells (1s, 2s and 2p) where 1s and 2s filled by two electrons for studied atoms and 2p has one   electron in B, two electrons in C, three electrons in N, four electrons in O, five electrons in F and six electrons in Ne. . All results in this study are calculated using   atomic unit, and found by computer program called Mathcad 2001i professional

Figure 1 represents the relation between one-particle radial density distribution function with the atomic number and we notice in this figure whenever the atomic number increases the maximum value of of one-electron radial density distribution function increases, also whenever the intra shell approached the nucleus for specific atom the maximum value increases too, in this figure we notice there is two peak in 2s and this according to effect called the penetration.

From the linkage between the one-electron radial density distribution function with the one-electron expectation value and as we notice in **table 1** the increasing in atomic number making the one-electron expectation value   when $k = -2, -1$ increases and when $k = 1, 2$ decrease.

The attraction potential for each individual shell and the total attraction potential for   each studied systems calculated   by equation (9) from this equation we notice the linkage between the attraction potential and one-electron expectation value when $k = -1$. Form

Table 2 we notice the increasing in atomic number causing increase attraction potential according to Coulomb's law where the increasing of the number of electron in each specific shell   and the decreasing in the distance between the nucleus and the intra shell causing increase in attraction potential for that shell. That explains the inequality in contribution ratio of the attraction potential in the total attraction potential for all intra shells as we see in **figure 2**.

-A-

-B-

-C-
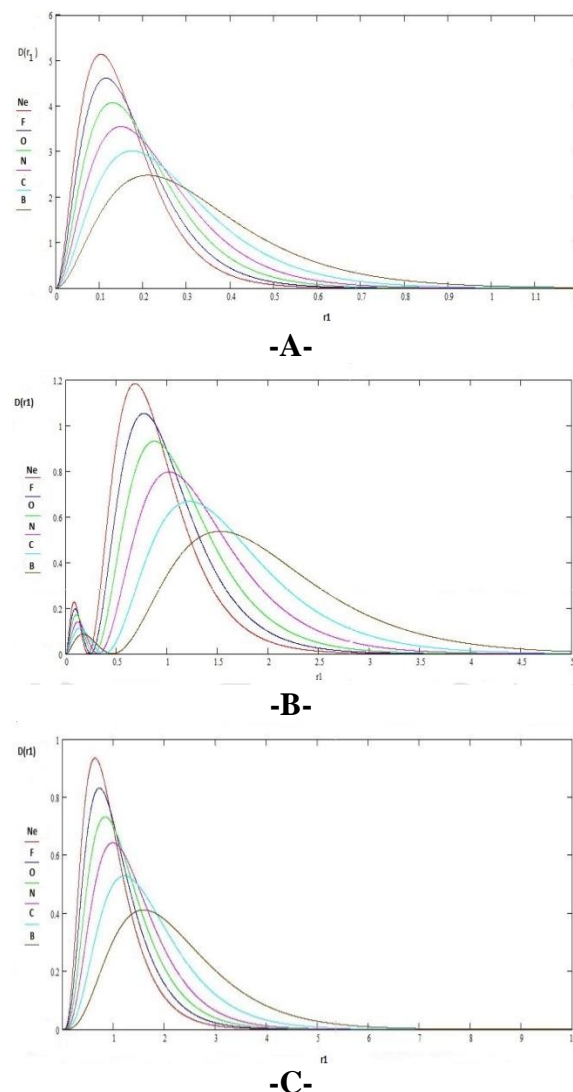
Figure 1: The relation between one-electron radial density distribution function with the atomic number for each individual atom;

**-A for 1s   -B- for 2s   -C- for 2p.**

Table 1: Results of one-particle expectation values for $-2 \leq k \geq 2$ and the standard deviation

Atoms			$< r_n^{-2} >$	$< r_n^{-1} >$	$< r_n^1 >$	$< r_n^2 >$	Δr_1
B	1S	Present w.	44.4445	4.66873	0.32668	0.14451	0.19438
		Ref. 10	44.538	4.674	0.325	0.143	-
	2S		2.11631	0.72062	1.96778	4.66319	0.88940
	2P		0.52989	0.60501	2.20476	6.14607	1.13363
C	1S		65.11471	5.66041	0.26872	0.09753	0.15913
	2S		3.35508	0.90284	1.58505	3.03670	0.72410
	2P		0.89207	0.78350	1.71449	3.74680	0.89850
N	1S	Present w.	89.76268	6.65196	0.22835	0.07035	0.13493
		Ref. 10	89.841	6.653	0.228	0.070	-
	2S		4.81216	1.08203	1.32866	2.13753	0.61008
	2P		1.33629	0.95769	1.40963	2.54764	0.74872
O	1S		118.23011	7.63785	0.19875	0.05328	0.11700
	2S	Present w.	6.71906	1.27338	1.13601	1.56314	0.52213
		Ref. 14	6.59145	1.26527	1.14196	1.58122	-
	2P		1.81872	1.11111	1.23220	1.97497	0.67577
F	1S	Present w.	150.76068	8.62941	0.17579	0.04166	0.10373
		Ref. 14	150.83417	8.63036	0.17574	0.04161	-
	2S	Present w.	8.70620	1.44715	1.00349	1.22311	0.46488
		Ref. 15	8.69721	1.44975	1.00109	1.21656	-
	2P		2.39477	1.27167	1.08479	1.54352	0.60561
Ne	1S	Present w.	187.27378	9.61756	0.15770	0.03351	0.09297
		Ref. 15	187.19696	9.61805	0.15763	0.03347	-
	2S	Present w.	11.09484	1.63274	0.89225	0.96741	0.41388
		Ref. 14	11.07131	1.63255	0.89211	0.96708	-
	2P		3.05886	1.43535	0.96526	1.22849	0.54473

Table 2: The expectation value of attraction potential for each individual shell

Atom	Shell		$-< Ven >$
B	1S	Present w.	46.6873
		Ref. 13	46.6873
	2S	Present w.	7.20620
		Ref. 11	7.12887
	2P		3.02505
	Total		**56.9186**
C	1S	Present w.	67.92492
		Ref. 13	67.92492
	2S	Present w.	10.83408
		Ref. 11	10.7614
	2P		9.40200
	Total		**90.1611**
	1S		93.12744

	2S	15.14842
N	2P	20.11149
	Total	**128.387**
O	1S	122.20560
	2S	20.37408
	2P	35.55552
	Total	**178.135**
F	1S	155.32938
	2S	26.04870
	2P	57.22515
	Total	**238.603**
Ne	1S	192.35120
	2S	32.65480
	2P	86.12100
	Total	**311.127**
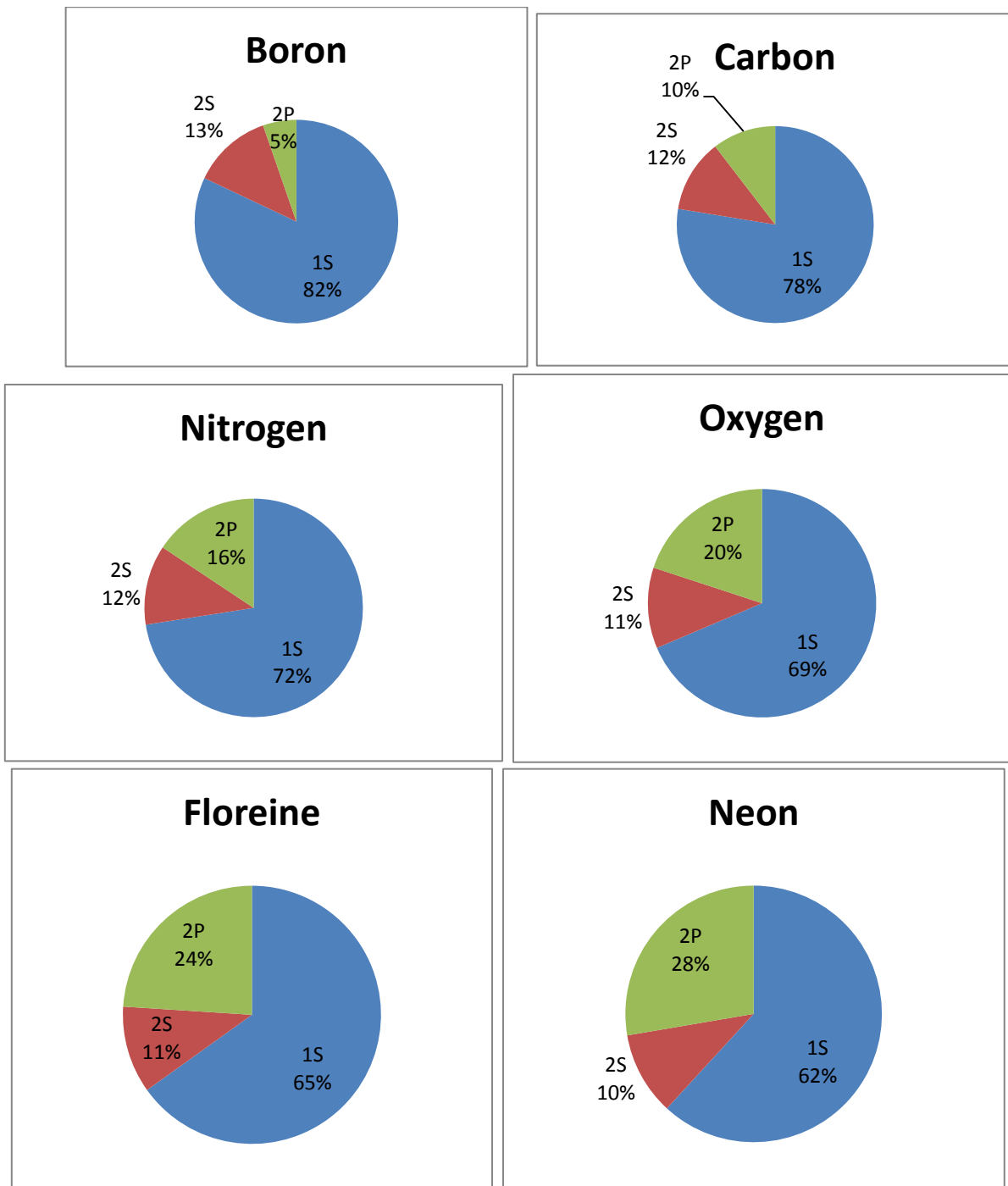
Figure 2: The ratio between the attraction energy of each intra shells relative to the total attraction energy of intra shells.

4. Conclusions

1. The attraction potential of **1s** shell is biggest value than **2s** and **2p** shells for each individual atom, also the **2s** have a bigger value than **2p** in Boron and Carbon atoms but when the number of electron in **2p** increased above the **2s** shell in this moment the attraction potential in **2p** shell be bigger than **2s.**

2. The total attraction potential increase when atomic number increase**.**

5. Reference

[1] R. Fitzpatrick, Quantum Mechanics, 3rd edition, 2011.

[2] A. Bunge , J. Chem. Phys. , Vol. 53, 1970.

[3] B. Goddard, Ph.D. thesis, Mathematical Analysis of Quantum Chemical Models for small atoms, 2007.

[4] K. Al-Bayati et., J. of Baghdad for science, Vol. 11, No. 4, 2014.

[5] K. Al-Bayati et., J. of Baghdad for science, vol. 11, No. 2, 2014.

[6] R. J. Boyd, Can. J. Phys., Vol.53, 1975.

[7] T. Koga, J. Theor. Chem. Acc., Vol. 118, 2007.

[8] K. Al-Khafaji, Sh. A. Kadhim and A. Al-Shebly, J. Karbala Univ., Vol. 6, No. 1,2008.

[9] S. Gldal, M.Sc. thesis, First Principle Study of The Sito occupancy and Magnetic Properties of Zinc-Tin Substituted Strontium Hexaferrite, Mississippi State Univ., 2011.

[10] B. Hassan   and K.Al-Bayati, J. Baghdad for Science, Vol. 7, No. 1, 2011.

[11] Sh. A. Kadhim, Iraqi J. of Phys., Vol. 11, No. 22, 2013.

[12] E. Al-Hatajawi, M.Sc. thesis, A Study of Some Atomic Properties for He-like Ions by Using Hartree-Fock Wavefunction, Kufa Univ., 2011.

[13] A. Mohammed, M.Sc. thesis, Calculation of The Energies of K-shell for Some Atoms by using Hartree-Fock Wavefunction, 2013.

[14] Saito, Atomic Data and Nuclear Data Tables, Vol. 95, 2009.

[15] C. F. Bunge and J. A. Barrientos, Atomic Data and Nuclear Data Tables, Vol. 53, 1993.