

A study of some Atomic properties for B - like ions of by using Hartree-Fock wave function.

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Abstract:

We studied some atomic properties of the like ions of the Beryllium atom (B^{+1} , C^{+2} and N^{+3} ions) in the closed shells by using Hartree – Fock (HF) wave function, so we calculated Hartree – Fock energy HF (non – relativistic energy) by using Math CAD (professional 2001i) where ($B^{+1}= 24.238$ hartree, $C^{+2}= 36.408$ hartree and $N^{+3}=51.0832$ hartree). Then compared these results with some experimental results.

Key words: Atomic properties , B - like ions , Hartree-Fock

دراسة الخواص الذرية للأيونات الشبيهة بذرة البريليوم باستخدام دالة هارترى – فوك

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الخلاصة :

درست بعض الخواص الذرية للأيونات الشبيهة بذرة البريليوم باستخدام دالة هارترى – فوك وحسبت طاقة هارترى – فوك (الطاقة الغير نسبية) لأيون البورون وأيون الكربون وأيون ألنتروجين وكانت قيم ($B^{+1}= 24.238$, $C^{+2}= 36.408$, $N^{+3}= 51.0832$) ووجدت متوافقه مع النتائج العمليه المنشوره سابقا.

كلمات مفتاحية: الخواص الذرية ، ذرة البريليوم ، هارترى – فوك

1. Introduction

In 1926 Erwin Schrodinger developed an equation, called a wave equation, to describe the behavior of matter wave. By using Schrodinger's equation scientists can find the wave function which solves a particular problem in quantum mechanics. Unfortunately, it is usually impossible to find an exact solution to the equation, so certain assumptions are used in order to obtain an approximate answer for the particular problem.[1]

Hartree – Fock theory was developed to solve the electronic Schrodinger equation that results from the time-independent Schrodinger equation after invoke the Born-Oppenheimer approximation. Hartree – Fock theory is fundamental for much of electronic structure theory. It is the basis of molecular orbital (MO) theory, which posits that each electron's motion can be described by a single-particle function (orbital) which does not depend explicitly on the instantaneous motions of the other electrons. It is always important to remember the context of a theory.

The basic idea of Hartree-Fock theory is as follows. We know how to solve the electronic problem for the simplest atom, hydrogen, which has only one electron. We imagine that perhaps if we added another electron to hydrogen, to obtain H^{-1} , then maybe it might be reasonable to start off pretending that the electrons don't interact with each other (i.e., that $V_{ee} = 0$). If that is true, then the Hamiltonian would be separable, and the total electronic wavefunction $\Psi(r_1, r_2)$ describing the motions of the two electrons would just be the product of two hydrogen atom wave functions (orbitals), $\Psi_H(r_1) \Psi_H(r_2)$. [2]

2. Theory

In classical mechanics the forces on a system creates two kinds of energy kinetic and potential. The Hamiltonian operator H is therefore broken into two operators, one represents kinetic energy (T) and other represents potential energy (V).[3]

$$H = T + V \quad \dots\dots\dots(1)$$

Where T is the kinetic energy :[4]

$$T = T_e + T_n \quad \dots\dots\dots(2)$$

T_e is the kinetic energy for electron = $-\frac{1}{2} \sum_i \nabla_i^2$

T_n is the kinetic energy for nucleus = $-\frac{1}{2M_a} \sum_a \nabla_a^2$

∇^2 is the Laplacian.

And V is potential energy :

$$V = V_{nn} + V_{en} + V_{ee} \quad \dots\dots\dots(3)$$

V_{nn} is the nuclear-nuclear repulsion term = $\sum_{A < B} \frac{Z_A Z_B}{R_{AB}}$

V_{en} is the nuclear-electron attraction term = $\sum_{iA} \frac{Z_A}{R_{iA}}$

V_{ee} is the electron-electron repulsion term = $\sum_{i < j} \frac{1}{r_{ij}}$

The Born-Oppenheimer approximation clamps the nuclei and implies

$$T_n = 0 \text{ and } V_{nn} \text{ is constant.}$$

This mean the Hamiltonian equation become.[5]

$$H = T_e + T_n + V_{nn} + V_{en} + V_{ee} \dots\dots(4)$$

$$H = -\frac{1}{2}\sum_{i=1}^n \nabla_i^2 - \sum_{i=1}^n \frac{z}{r_i} + \sum_{i=1}^{n-1} \sum_{j=i+1}^n \frac{1}{r_{ij}} \dots\dots\dots(5)$$

Then we are led to the idea of the Slater determinant for the trial wave functions. We can write a Slater determinant:[6]

$$\Phi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\vec{x}_1) & \phi_2(\vec{x}_1) & \dots & \phi_N(\vec{x}_1) \\ \phi_1(\vec{x}_2) & \phi_2(\vec{x}_2) & \dots & \phi_N(\vec{x}_2) \\ \vdots & \vdots & & \vdots \\ \phi_1(\vec{x}_N) & \phi_2(\vec{x}_N) & \dots & \phi_N(\vec{x}_N) \end{vmatrix} \dots\dots\dots(6)$$

The factor $\frac{1}{\sqrt{N!}}$ Is normalization factor. This Slater determinant has N electrons occupying N spin orbitals($\phi_1, \phi_2, \dots, \phi_N$) without specifying which electron is in which orbital.

Generally, such a determinant can be simply represented with only the diagonal elements as given below:

$$\Phi = \hat{A}[\phi_1(1). \phi_2(2) \dots \dots \phi_N(N)] = \hat{A}\Pi \dots\dots\dots(7)$$

Where Π is the determinant diagonal product and \hat{A} is the antisymmetrizer:

$$\hat{A} = \frac{1}{\sqrt{N!}} \sum_{p=0}^{N-1} (-1)^p \hat{P} \dots\dots\dots(8)$$

\hat{P} is a permutation operator, \hat{P}_{ij} permutes two electrons, \hat{P}_{ijk} permutes three electrons, and so on.[7]

Where spin-orbital function:

$$\phi_{nl} = \sum_{i=1}^j C_n^i x_{nlm}^i \dots\dots\dots(9)$$

Where n, l, m is the quantum numbers.

C_n^i represent the constant coefficient, and x_{nlm}^i is the basis function as a standard normalization Slater type orbital (STO'S) is equal to:

$$x_{nlm}(\vec{r}, \vec{\xi}) = R_{nl}(r, \xi) Y_{lm_l}(\theta, \phi) \dots\dots\dots(10)$$

Where $R_{nl}(\vec{p})$ is the radial factor which describes how the wave function ϕ of the electron varies with the radial distance from the nucleus and the angular factor $Y_{lm_l}(\theta, \phi)$. [8]

$$R_{nl}(r, \xi) = N_{nlm_l} S_{nl}(r) \dots\dots\dots(11)$$

Where N_{nlm_l} is the normalization constant given by:[9.10]

$$N_{nlm_l} = \frac{(2\xi)^{n+\frac{1}{2}}}{[(2n)!]^{\frac{1}{2}}} \dots\dots\dots(12)$$

$$S_{nl}(r) = r^{n-1} e^{-\xi.r} \dots\dots\dots(13)$$

Where ξ the orbital exponent is related directly to the nuclear charge of the hydrogenic atom in the equation.[9]

$$\xi = \frac{z}{n} \dots\dots\dots(14)$$

Where $S_{nl}(r)$ is the radial part of STO'S. Where z is the nuclear charge, in the case of the hydrogenic system, only one electron is associated with the system and therefore the electron will always feel the full in the nuclear charge (that is, there is no nuclear shielding due to the presence of other electrons).

The two – electron radial density function $D(r_1, r_2)$ given by:

$$D(r_1, r_2) = r_1^2 r_2^2 \int \int \Gamma(r_1, r_2) d\Omega_1 d\Omega_2 \dots\dots\dots(15)$$

$$\Gamma(r_1, r_2) = \frac{N(N-1)}{2} \int |\psi(r_1, r_2, r_N)|^2 dx_3 dx_N ds_1 ds_2 \dots\dots\dots(16)$$

The function $D(r_1, r_2)$ is the probability density that one electron is at radius r_1 and the

other electron at radius r_2 when any two electron are considered simultaneously.[10]

The one – electron radial density distribution function $D(r_1)$ is of finding an electron at a distance r from the coordinate origin.[11]

$$D(r_1) = \int_0^\infty D(r_1, r_2) dr_2 \dots (17)$$

The inter-particle distribution function associated with the spin-orbital pair(i,j) is given by [12]

$$f(r_{12}) = \int \Gamma(r_1, r_2) dr_1 dr_2 \quad (18)$$

The one – electron expectation value $\langle r_1^m \rangle$ where $-2 \geq m \geq 2$ in this research, it is determined by the expression as: [13]

$$\langle r_1^m \rangle = \int_0^\infty D(r) r_1^m dr_1 \dots (19)$$

The inter – electron expectation value $\langle r_{12}^m \rangle$ where $-2 \geq m \geq 2$ in this research, it is determined by the expression as:

$$\langle r_{12}^m \rangle = \int_0^\infty f(r_{12}) r_{12}^m dr_{12} \dots (20)$$

The standard deviation of distance of the test electron from the nucleus r_1 is defined as[14].

$$\Delta r_1 = \sqrt{\langle r_1^2 \rangle - \langle r_1 \rangle^2} \dots (21)$$

While the standard deviation of the inter electronic distance of the two electrons, is defined as[15].

$$\Delta r_{12} = \sqrt{\langle r_{12}^2 \rangle - \langle r_{12} \rangle^2} \dots (22)$$

The total energy is defined by.[16]

$$E = T + V_{ee} + V_{en} \dots (23)$$

T is the kinetic energy, V_{ee} is the coulomb repulsion between electron – electron, and V_{en} is an attraction energy between electron – nucleus, of the expectation value of the kinetic and potential energies given by:

$$\langle T \rangle = -\frac{1}{2} \int \psi * [\sum_i^N \nabla_i^2] \psi d\tau$$

$$V_{ee} = \int \psi * \sum_{i>j}^N \frac{1}{|r_i - r_j|} \psi d\tau$$

$$V_{en} = \int \psi * \sum_i^N -\frac{Z}{r_i} \psi d\tau$$

$$\langle V \rangle = -Z \langle \frac{1}{r_1} \rangle + \langle \frac{1}{r_{12}} \rangle \quad (16)$$

The expectation value for energy is defined as:

$$\langle E \rangle = \frac{1}{2} \langle V \rangle \dots (24)$$

Result and discuses (17)

We used the atomic data for Hartree-fock function for iso-electronic of Be-atom Clementi and Roetti. [17]

Table(1) parameters of the ions. (18)

A		B ⁺ – ion	
n	ζ	c ₁	c ₂
1	4.42994	0.92801	-0.20288
1	7.86336	0.08063	-0.01942
2	1.59241	0.00320	0.73490
2	4.01022	-0.00081	-0.09218
2	1.25021	-0.00198	0.34527
B		C ⁺⁺ – ion	
n	ζ	c ₁	c ₂
1	5.43806	0.94114	-0.23411
1	9.62456	0.06483	-0.01534
2	2.05179	0.00453	0.81829
2	4.72768	0.00033	-0.11736
2	1.72221	-0.00313	0.28540
C		N ⁺⁺⁺ – ion	
n	ζ (21)	c ₁	c ₂
1	6.45100	0.94954	-0.25378
1	11.38700	0.05374	-0.01283
2	2.50371	0.00616	0.86016
2	5.53122	0.00230	-0.13747
2	2.25623	-0.00486	0.26208

The atomic properties such as inter-particle distribution function $f(r_{12})$, one-particle radial distribution function $D(r_1)$ and all expectation values $\langle r_1^m \rangle \langle r_{12}^m \rangle \langle V \rangle \langle T \rangle \langle E \rangle$ were obtained numerically by using Mathcad 2001i.

We calculated the one-particle radial density function by using equation (17) , table(2) indicated the maximum values of the $D(r_1)$ and values of the positions and inter – electron distribution function $f(r_{12})$ by using equation (18) and table(3) , from these results we noticed when the atomic number increased the maximum values of $D(r_1)$ and $f(r_{12})$ was increasing and the values of the position decreased because the effect of nuclear charge increased, From fig(1) to Fig(7) show the relation between $D(r_1)$ and position we found when $r_1 = 0$; $D(r_1) = 0$ and when $r_1 = \infty$, $D(r_1) = 0$ that means the electron was not found in the nucleus or out the orbitals.

The probability of finding the electron in the K – shell is large than those in the L – shell and $K_\alpha L_\beta$ –shell, $K_\alpha L_\alpha$ – shell, $K_\beta L_\beta$ –shell and $K_\beta L_\alpha$ –shell because K – shell closer to nuclear from other shell, and the probability of finding the electron in L – shell is large than those in the $K_\alpha L_\beta$ –shell, $K_\alpha L_\alpha$ –shell, $K_\beta L_\beta$ –shell and $K_\beta L_\alpha$ –shell because L – shell is far to the nucleus from other shell this mean the attraction energy the nucleus for this shell is larger than the attraction energy the nucleus for other shells and the probability of finding the electron $K_\alpha L_\beta$ –shell, $K_\alpha L_\alpha$ –shell, $K_\beta L_\beta$ –shell and $K_\beta L_\alpha$ –shell is similar because are have some r_1 .

we noted from fig(2) and (3):

There are two peaks for L – shell, $K_\alpha L_\beta$ –shell, $K_\alpha L_\alpha$ – shell, $K_\beta L_\beta$ –shell and $K_\beta L_\alpha$ – shell. The first peak represents the probability of finding the electron in the K – shell, the second peak represents the probability of finding the electron in the L – shell this appear in fig (3) and we see that the first peak is large than the second peak because K – shell is closer to the nucleus than L – shell, so that attraction force between the nucleus and the electron is large for K – shell than for L – shell according to coulomb law but in fig(2) the first peak smaller from second peak because the first peak represent the probability finding the electron in the small

distance and the second peak represent the probability finding the electron in the large distance, and this figure represent the probability find the electron between two shell is less.

We noted from fig(4), (5), (6) and (7)

One peak in the K-shell, L-shell, ($K_\alpha L_\beta$, $K_\alpha L_\alpha$, and $K_\beta L_\beta$) shell and two peak in the $K_\beta L_\alpha$ –shell because in the $K_\beta L_\alpha$ –shell the electron β in the K-shell non associated with the electron α in the L-shell, so the two electrons are anti-parallel (has the different spin $(+\frac{1}{2}, -\frac{1}{2})$) and according to Pauli exclusion principle (no two electrons can occupy the same spin state) therefore, there is one probability of finding two electrons non simultaneous in the $K_\beta L_\alpha$ –shell two peaks, the first peak indicates the probability of finding two electron in small distance r_{12} and the second peak represented the probability of finding two electron in the larger distance between them(r_{12}).

inter – electron expectation value $\langle r_{12}^m \rangle$ from table(3) :When $m = -1, -2$ the inter – electron expectation value $\langle r_{12}^m \rangle$ increases as atomic number increases, when $m = 1, 2$ the inter – electron expectation value decreases when atomic number increases.

For K-shell, the values of $\langle r_{12}^m \rangle$ when $m = -1, -2$ are greater than those in L-shell, ($K_\alpha L_\beta$, $K_\alpha L_\alpha$, $K_\beta L_\beta$ and $K_\beta L_\alpha$) shell, and when $m = 1, 2$ the values of $\langle r_{12}^m \rangle$ for K-shell are smaller than those in L-shell, ($K_\alpha L_\beta$, $K_\alpha L_\alpha$, $K_\beta L_\beta$ and $K_\beta L_\alpha$) shell because K-shell closer to the nucleus from other shells.

Table(2): values of positions and maximum values of the $D(r_1)$ for studied systems for all shell.

shell		B^{+1}	C^{+2}	N^{+3}	
K	r_1	0.21	0.17	0.15	
	$D_{max}(r_1)$	2.4848	3.0230	3.5647	
L	Peak 1	r_1	0.17	0.14	0.12
		$D_{max}(r_1)$	0.0992	0.1479	0.1976
	Peak 2	r_1	1.45	1.13	0.92
		$D_{max}(r_1)$	0.6020	0.8016	0.9980
$K_\beta L_\alpha$ $\equiv K_\alpha L_\alpha$ $\equiv K_\beta L_\beta$ $\equiv K_\alpha L_\beta$	Peak 1	r_1	0.21	0.17	0.15
		$D_{max}(r_1)$	1.2885	1.5807	1.8720
	Peak 2	r_1	1.44	1.12	0.91
		$D_{max}(r_1)$	0.3019	0.4027	0.5021

Table (3): The maximum values of the $f(r_{12})$ and corresponding values for studied systems for all shells.

shell		B^{+1}	C^{+2}	N^{+3}	
K	r_{12}	0.36	0.29	0.25	
	$f(r_{12})$	1.8218	2.2186	2.6169	
L	r_{12}	2.25	1.73	1.41	
	$f(r_{12})$	0.3741	0.4916	0.6071	
$K_\alpha L_\alpha$ $\equiv K_\beta L_\beta$ $\equiv K_\alpha L_\beta$	r_{12}	1.50	1.16	0.95	
	$f(r_{12})$	0.5760	0.7614	0.9435	
$K_\beta L_\alpha$	Peak 1	r_{12}	0.29	0.24	0.20
		$f(r_{12})$	0.1074	0.1587	0.2111
	Peak 2	r_{12}	1.52	1.19	0.98
		$f(r_{12})$	0.5822	0.7677	0.9490

Fig (1): the relation between one electron radial density function $D(r_1)$ and the position (r_1) for K-shell.

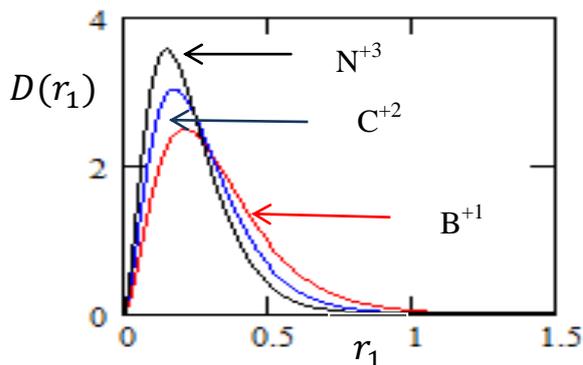


Fig (2): The relationship between one electron radial density function $D(r_1)$ and the position (r_1) for L-shell.

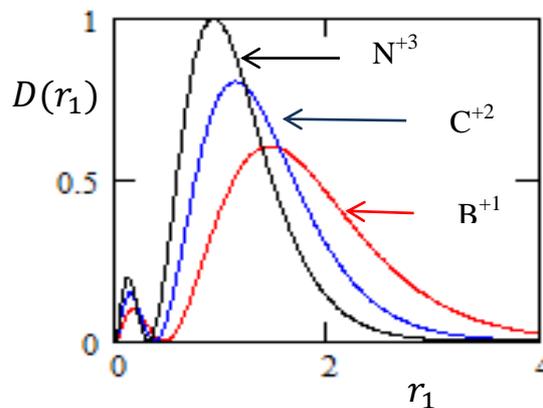


Fig (3): the relation between one electron radial density function $D(r_1)$ and the position (r_1) for $K_\alpha L_\beta$ shell, $K_\beta L_\alpha$ shell, $K_\alpha L_\alpha$ shell and $K_\beta L_\beta$.

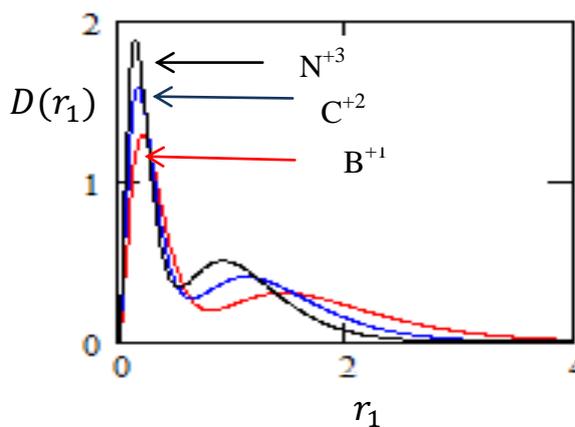


Fig (4): The relationship inter-particle distribution function and r_{12} for K-shell of four electron systems.

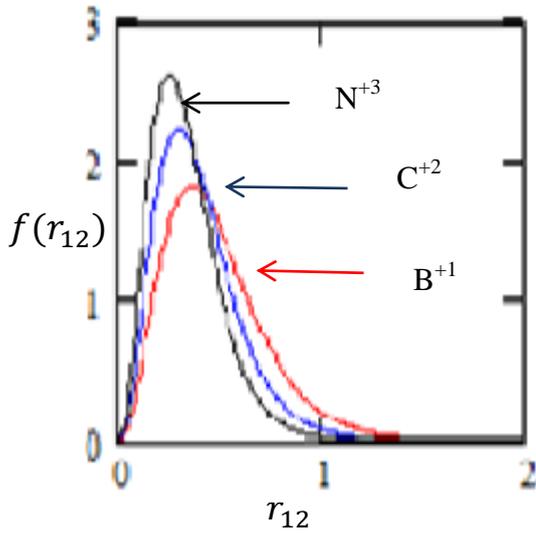


Fig (6): The relationship inter-particle distribution function and r_{12} for $K_{\alpha}L_{\beta}$ shell, $K_{\alpha}L_{\alpha}$ shell and $K_{\beta}L_{\beta}$ shell of four electron systems.

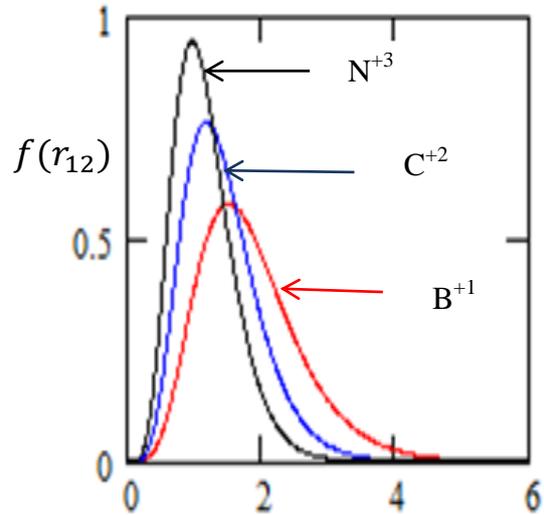


Fig (5): The relationship inter-particle distribution function and r_{12} for L-shell of four electron system.

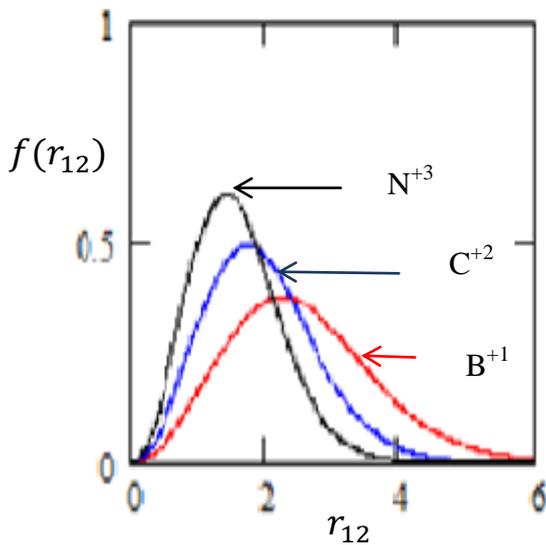
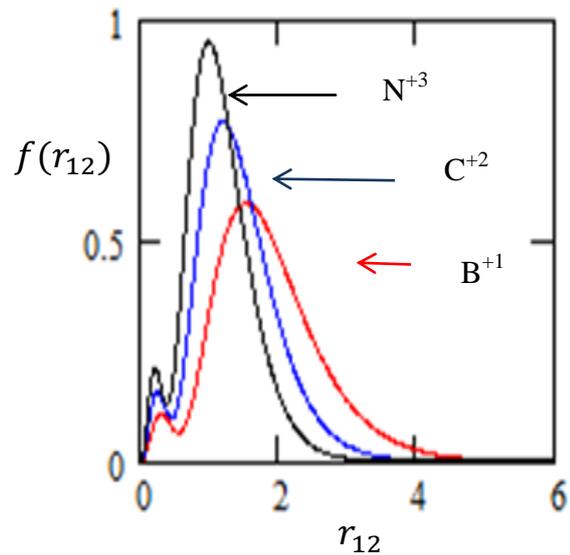


Fig (7): The relationship inter-particle distribution function and r_{12} for $K_{\beta}L_{\alpha}$ shell of four electron systems.



For L-shell, the value of $\langle r_{12}^m \rangle$ when $m=-1,-2$ are less than those in K-shell, ($K_\alpha L_\beta$, $K_\alpha L_\alpha$, $K_\beta L_\beta$ and $K_\beta L_\alpha$) shell, and when $m=1,2$ the value of $\langle r_{12}^m \rangle$ for L-shell are greater than those in K-shell, ($K_\alpha L_\beta$, $K_\alpha L_\alpha$, $K_\beta L_\beta$ and $K_\beta L_\alpha$) shell because L-shell far to the nucleus from other shell. The value of $\langle r_{12}^m \rangle$ when $m=-1,-2$ in the $K_\beta L_\alpha$ - shell is greater than those in the ($K_\alpha L_\beta$, $K_\alpha L_\alpha$ and $K_\beta L_\beta$) shell because the two electron in the $K_\beta L_\alpha$ -shell are anti-parallel so the $\langle r_{12}^m \rangle$ (which represent the repulsion energy between two electron) is larger in the $K_\beta L_\alpha$ -shell. The value of $\langle r_{12}^m \rangle$ when $m=1,2$ in the $K_\beta L_\alpha$ - shell is less than those in the ($K_\alpha L_\beta$, $K_\alpha L_\alpha$ and $K_\beta L_\beta$) shell because the two electron in the $K_\beta L_\alpha$ -shell had different spin ($+\frac{1}{2}, -\frac{1}{2}$) so the distance must be small between them.

The inter – electron expectation value $\langle r_{12}^m \rangle$ equal to unity for all system when $m=0$, Standard deviation for studied systems decreases when atomic number increases. Standard deviation for K-shell is smaller than those in L-shell, ($K_\alpha L_\beta$, $K_\alpha L_\alpha$, $K_\beta L_\beta$ and $K_\beta L_\alpha$) shell, and standard deviation for ($K_\alpha L_\beta$, $K_\alpha L_\alpha$ and $K_\beta L_\beta$) shell is smaller than those in the L-shell and $K_\beta L_\alpha$ -shell, and standard deviation for $K_\beta L_\alpha$ -shell is smaller than those in the L-shell

The discusses for $\langle r_1^m \rangle$ some for $\langle r_{12}^m \rangle$ from table (4). distance between electrons with nucleus, as well as the distance between two electron, this product increasing in attraction energy and repulsion energy according to coulomb law. The expectation value of kinetic energy $\langle T \rangle$ when atomic number (Z) increases because when increasing in atomic number lead to increasing in the attraction energy this mean decreases the distance between nucleus and electron lead to increasing in the velocity

of the electron around the nucleus and decreasing in its radius and increasing in its kinetic energy $\langle T \rangle$. Expectation value of HF energy $\langle E_{HF} \rangle$ increases as atomic number increases because increasing in the potential energy and kinetic energy lead to increasing in the total energy of the system (HF energy). the expectation value of all energies in K-shell is laeger than those in the other shell because K-shell is closer to the nucleus than other shell. And the expectation value of all energies in L-shell is less than those in other shell because L-shell is far than those in other shell. It can be observe the expectation value of repulsion energy in the $K_\beta L_\alpha$ -shell is larger than that in the ($K_\alpha L_\beta$, $K_\alpha L_\alpha$ and $K_\beta L_\beta$) shell because the distance between two electrons in the $K_\beta L_\alpha$ -shell is smaller than that in the ($K_\alpha L_\beta$, $K_\alpha L_\alpha$ and $K_\beta L_\beta$) shell, and this lead to the expectation value of potential energy in the $K_\beta L_\alpha$ -shell is smaller than that in the ($K_\alpha L_\beta$, $K_\alpha L_\alpha$ and $K_\beta L_\beta$) shell we noted that from table (6).

For all studied systems, the expectation value of attraction energy $\langle V_{en} \rangle$ and expectation value of repulsion energy $\langle V_{ee} \rangle$ increases when atomic number increases because increasing in Z leads to decreasing in the

Table(4):The expectation values of r_{12} and standard deviation for each shell

<i>ions</i>	$\langle r_{12}^{-2} \rangle$	$\langle r_{12}^{-1} \rangle$	$\langle r_{12}^0 \rangle$	$\langle r_{12}^1 \rangle$	$\langle r_{12}^2 \rangle$	Δr_{12}
<i>B+1</i>	<i>K</i>	14.4395	2.8962	1	0.4756	0.2433
	<i>L</i>	0.4115	0.5038	1	2.5405	1.0944
	$K_{\beta}L_{\beta} \equiv K_{\alpha}L_{\alpha} \equiv K_{\alpha}L_{\beta}$	0.5406	0.6565	1	1.8372	0.7703
	$K_{\beta}L_{\alpha}$	1.4166	0.7487	1	1.8271	0.7939
	<i>Total</i>	2.9815	1.0197	1	1.7258	0.7395
<i>C+2</i>	<i>K</i>	21.2955	3.5199	1	0.3907	0.1994
	<i>L</i>	0.7081	0.6594	1	1.9363	0.8248
	$K_{\beta}L_{\beta} \equiv K_{\alpha}L_{\alpha} \equiv K_{\alpha}L_{\beta}$	0.9026	0.8512	1	1.4069	0.5759
	$K_{\beta}L_{\alpha}$	2.4740	0.9864	1	1.3971	0.5993
	<i>Total</i>	4.5309	1.2861	1	1.3241	0.5585
<i>N+3</i>	<i>K</i>	29.4841	4.1439	1	0.3317	0.1689
	<i>L</i>	1.0805	0.8128	1	1.5686	0.6640
	$K_{\beta}L_{\beta} \equiv K_{\alpha}L_{\alpha} \equiv K_{\alpha}L_{\beta}$	1.3508	1.0433	1	1.1432	0.4616
	$K_{\beta}L_{\alpha}$	3.8074	1.2219	1	1.1340	0.4838
	<i>Total</i>	6.4040	1.5514	1	1.0773	0.4505

Table(5):The expectation values of r_1 and standard deviation for each shell

<i>ions</i>	<i>shell</i>	$\langle r_1^{-2} \rangle$	$\langle r_1^{-1} \rangle$	$\langle r_1^0 \rangle$	$\langle r_1^1 \rangle$	$\langle r_1^2 \rangle$	Δr_1
<i>B+1</i>	<i>K</i>	44.6076	4.6792	1	0.3253	0.1427	0.1920
	<i>L</i>	2.4150	0.7801	1	1.7982	3.8259	0.7697
	$K_{\beta}L_{\beta} \equiv K_{\alpha}L_{\alpha} \equiv K_{\alpha}L_{\beta}$	23.5113	2.7297	1	1.0617	1.9843	0.9258
	$K_{\beta}L_{\alpha}$	23.5113	2.7297	1	1.0617	1.9843	0.9258
	<i>Total</i>	23.5113	2.7297	1	1.0617	1.9843	0.7776
<i>C+2</i>	<i>K</i>	65.4610	5.6773	1	0.2674	0.0962	0.1573
	<i>L</i>	2.2837	1.0341	1	1.3720	2.2148	0.5766
	$K_{\beta}L_{\beta} \equiv K_{\alpha}L_{\alpha} \equiv K_{\alpha}L_{\beta}$	34.8722	3.3557	1	0.8197	1.1555	0.6954
	$K_{\beta}L_{\alpha}$	34.8724	3.3557	1	0.8197	1.1555	0.6954
	<i>Total</i>	34.5389	3.3557	1	0.8197	1.1555	0.5856
<i>N+3</i>	<i>K</i>	90.3101	6.6759	1	0.2270	0.0693	0.1332
	<i>L</i>	6.6573	1.2866	1	1.1120	1.4507	0.4628
	$K_{\beta}L_{\beta} \equiv K_{\alpha}L_{\alpha} \equiv K_{\alpha}L_{\beta}$	48.4835	3.9812	1	0.6695	0.7600	0.5584
	$K_{\beta}L_{\alpha}$	48.4836	3.9812	1	0.6695	0.7600	0.5584
	<i>Total</i>	48.4839	3.9812	1	0.6695	0.7600	0.4713

Table (6): The expectation values for attraction, repulsion, kinetic and Hartree-Fock energies for all shells and the total studied systems.

<i>ions</i>	<i>shell</i>	$-\langle V_{en} \rangle$	$\langle V_{ee} \rangle$	$-\langle V \rangle$	$\langle T \rangle$	$-\langle E_{HF} \rangle$	$-\langle E_{HF} \rangle$ Ref [17]
<i>B+1</i>	<i>K</i>	46.7920	2.8962	43.8958	21.9479	21.9479	24.2376
	<i>L</i>	7.8010	0.5038	7.2972	3.6486	3.6486	
	$K_{\alpha}L_{\beta} \equiv K_{\alpha}L_{\alpha} \equiv K_{\beta}L_{\beta}$	0.6565	0.6565	0.3282	0.3280	
	$K_{\beta}L_{\alpha}$	0.7487	0.7487	0.3744	0.3744	
	<i>total</i>	54.5930	6.1167	48.4748	24.2374	24.2374	
<i>C+2</i>	<i>K</i>	68.1276	3.5199	64.6077	32.3039	32.3039	36.4084
	<i>L</i>	12.4092	0.6594	11.7490	5.8745	5.8745	
	$K_{\alpha}L_{\beta} \equiv K_{\alpha}L_{\alpha} \equiv K_{\beta}L_{\beta}$	0.8512	0.8512	0.4251	0.4251	
	$K_{\beta}L_{\alpha}$	0.9864	0.9864	0.4932	0.4932	
	<i>total</i>	80.5368	7.7179	72.8167	36.4083	36.4083	
<i>N+3</i>	<i>K</i>	93.4626	4.1439	89.3187	44.6594	44.6594	51.0823
	<i>L</i>	18.0124	0.8129	17.1995	8.5998	8.5998	
	$K_{\alpha}L_{\beta} \equiv K_{\alpha}L_{\alpha} \equiv K_{\beta}L_{\beta}$	1.0433	1.0433	0.5215	0.5215	
	$K_{\beta}L_{\alpha}$	1.2219	1.2219	0.6109	0.6109	
	<i>total</i>	111.4750	9.3077	102.1664	51.0832	51.0832	

Conclusions

1- When $r_1=0$ or $r_1 =\infty$ the values of $D(r_1)=0$ and when $r_{12}=0$ or $r_{12} =\infty$ the values of the $f(r_{12})=0$

2-As Z increased the maximum values of inter- particle distribution function $f(r_{12})$ and one- particle radial density distribution function $D(r_1)$ increased and the positions of

these maximum values decreased with Z increased. values and decrease for n positive values.

3- As Z increased the values of $\langle r_1 \rangle, \langle r_{12} \rangle$ increased for n negative values and decreased for n positive values.

4- For the systems the standard deviation $\Delta r_1, \Delta r_{12}$ decreased as Z increased.

5-As Z increased, all the energies increased for all systems.

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