A study of some atomic properties for He-like selected ions

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Abstract:

The atomic properties have been studied for He-like ions (He atom, Li^{+}, Be^{2+} and B^{3+}ions). These properties included, the atomic form factor *f(S)*, electron density at the nucleus $\rho(0)$, nuclear magnetic shielding constant σ_d and diamagnetic susceptibility χ ,which are very important in the study of physical properties of the atoms and ions.

For these purpose two types of the wave functions applied are used, the Hartree-Fock *(HF)* waves function (uncorrelated) and the Configuration interaction *(CI)* wave function (correlated). All the results and the behaviors obtained in this work have been discussed, interpreted and compared with those previously obtained.

Theory:

The atomic properties under investigation include the following:

- **The atomic form factor *f(S)***

A quantity f(S) is used to describe the "efficiency" of scattering of a given atom in a given direction, and it is defined as a ratio of amplitude: [1,2]

$$f(s) = \frac{\text{Amplitude of the wave scattered by an atom}}{\text{Amplitude of the wave scattered by one electron}} \quad \ldots(1)$$

Mathematically, the relation of X-ray form factor $f(S)$ to the electron distribution function $D(r)$ in the atom is expressed by the formula [3,4].

$$f(s) = \int_0^\infty D(r) \frac{\sin 4\pi sr}{4\pi sr} dr \quad \ldots(2)$$

Where: $4\pi S$ is called the momentum transfer, $\frac{\sin sr}{sr}$ is the spherical Bessel function of zero order $J_{n=0}$ [5,6]

and $S = \sin\theta / \lambda$

Since:

$$J_n = x^n \left(\frac{-1}{x}\frac{d}{dx}\right)^n \left(\frac{\sin x}{x}\right) \quad \ldots (3)$$

The one particle radial density distribution D (r1) can be defined as [7,8,9]

$$(r1) = \int \int \int \psi(r1)\, \psi(r1)\, \psi(r2)\, \psi(r2)\, dr2\, d\Omega 1\, d\Omega 2 \qquad (4)$$

Where

$$d\Omega_i = \sin\theta_i d\theta_i d\varphi_i$$

- **Electron density at the nucleus $\rho(0)$**

The electron density at the nucleus can be evaluated using the following form, [10]

$$\rho(0) = \left[\frac{D(r)}{4\pi r^2}\right]_{r \to 0} \quad \ldots(5)$$

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- **Nuclear magnetic shielding constant** σ_d

The nuclear magnetic shielding constant is determined from the formula [11]

$$\sigma = \frac{1}{3}\alpha^2 \left\langle \psi \left| \sum_{i=1}^{n} \frac{1}{r_i} \right| \psi \right\rangle \quad \ldots(6)$$

Where α is the fine-structure constant.

$\alpha = 7.29735308 \times 10^{-3}$

n represents the number of particle

- **Diamagnetic susceptibility** χ

The diamagnetic susceptibility is defined by [12,13]:

$$\chi = -\frac{1}{6}\alpha^2 \left\langle \psi \left| \sum_{i=1}^{n} r_i^2 \right| \psi \right\rangle \quad \ldots(9)$$

Results and Discussion

1. The electron density at the nucleus $\rho(0)$:

Table (1) and Fig (1) show the results of the electron density at the nucleus $\rho(0)$ obtained by Hartree Fock and correlated wave functions for He - like ions. It is clear from the results that the effect of the atomic number upon the electron density, where the density increases by increasing the atomic number Z, this is due to the effect of the Coulomb attraction forces.

2. The atomic form factor f(S):

It is clear from Table (2) and Fig (2) show that the results of the behavior of atomic form factor starts from the maximum value, (at zero angle) equal to the atomic number that characterized each element or equal to the number of electrons for each shell, and gradually decline with increasing the scattering angle until reach to the minimum value. These maximum and minimum values are different from an element to another. Physically the maximum value of atomic form factor means that the full scattering of x-rays is occurred since all scattering rays in forward direction ($\theta = 0$) from the electrons of different locations are in the same phase because of their equal light pathways, so that, amplitude of scattering beam equals to the amplitude of scattering waves resulting from one electron multiplied by the atomic number Z.

According to this, increasing of the scattering the angle lead to increase of the light differences pathways between the scattered waves from the different electrons. This leads to partial distractive interference and decreasing in the total amplitude of the scattered wave associated with increasing the scattering angle and the minimum value means that the lowest scattering of x-rays is occurred also, where the path differences between the scattered waves by different location electrons are very large which results in more probability for occurrence of distractive interference which produces final resultant amplitude of small value.

3. Nuclear Magnetic Shielding σ_d and Diamagnetic Susceptibility χ

Table (3) shows that the nuclear magnetic shielding constant increases as Z decreases, this is due to the attraction force between the electrons and protons. Whereas the diamagnetic susceptibility decreases as Z increases as shown in table (4).

Conclusions:

From these results we can conclude several important points as:

1.The largest relative effects on x-ray scattering factor for the shell of smallest effective nuclear charge and greatest radius in an atom.

2.The maximum value of the form factor is obtained when the scattering angles is maximum (i.e. θ=0) which mean that the full scattering of x-rays is occurred.

3.The atomic scattering factor is very important to evaluate the nuclear magnetic shielding constant.

4.The nuclear magnetic shielding constant increases by increasing the atomic number (Z) but the diamagnetic susceptibility decreases by increasing the atomic number.

Table (1) Electron density at the nucleus ρ (0) for He like ions. Using HF Weiss CI wave function

Z	$\rho(0)$	
	HF	CI
2	3.596	4.001
3	13.683	15.516
4	34.408	39.351
5	63.375	69.536

Table (2) The varying of atomic form factors for He like ions with scattering angels.

$\sin\theta/\lambda$	$f(\sin\theta/\lambda)$							
	He		Li^{+}		Be^{+2}		B^{+3}	
	HF	CI	HF	CI	HF	CI	HF	CI
0.0	2	2	2	2	2	2	2	2
0.2	0.9784	1.0489	1.3220	1.3593	1.5912	1.6139	1.7326	1.7329
0.4	0.3060	0.3567	0.5627	0.6252	0.9181	0.9772	1.1928	1.1998
0.6	0.1188	0.1373	0.2338	0.2726	0.4762	0.5357	0.7298	0.7461
0.8	0.0567	0.0641	0.1063	0.1251	0.2493	0.2903	0.4323	0.4557
1	0.0318	0.0355	0.0532	0.0622	0.1369	0.1617	0.2591	0.2782

Table (3) Nuclear magnetic shielding constants for He-like ions, these results are derived using Weiss CI and HF wave functions

Z	σ_d	
	HF	CI
2	5.99-05	6.286-05
3	9.54-05	10.05-05
4	13.09-05	13.79-05
5	16.64-05	17.52-05

Table (4) Diamagnetic susceptibility for He-like ions, these results are derived using Weiss CI and HF wave functions

Z	χ	
	HF	CI
2	21.03-06	20.80-06
3	7.904-06	7.581-06
4	4.115-06	3.916-06
5	2.518-06	2.401-06

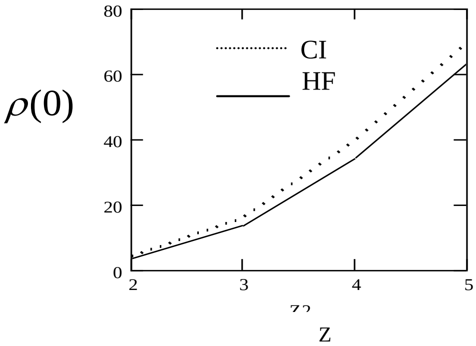

Fig (1) Electron density at the nucleus for He like selected ions using HF and CI wave function

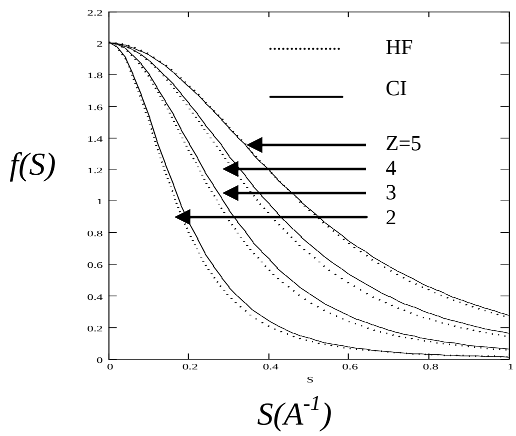

Fig (2) Comparison between the form factors of (He atom,Li^{+},Be^{2+},B^{3+} ions) using HF and CI wave functions.

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دراسة بعض الصفات الذرية للايونات الشبيهة للهليوم

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الخلاصــة:

تم دراسة بعض الصفات الذرية للايونات الشبيهة بالهليوم (ذرة الهليوم , ايونات Li^+ Be^{2+} , B^{3+}). هذه الصفات تتضمن عامل الاستطارة الذري , كثافة الإلكترون في النواة و ثابت الحجب النــووي المغناطيســي والقابلية الدايامغناطيسية والتي تعتبر جميعها مهمة في دراسة الصفات الفيزياوية في الذرات والايونـــات . لهـــذا الغرض تم تطبيق نوعين من الدوال الموجية النوع الأول هو دالة هارتري فوك والنوع الثاني دالـــة التفـــاعلات المنسقة جميع النتائج والعلاقات المستحصلة في هذا العمل تم مناقشتها وتفسيرها ومقارنتها مع النتائج المنشـــورة سابقا