Study of atomic properties in K-Shell for Na^{9+}, Mg^{10+}, Al^{11+} ions in position space

Entessar Farhan Selman
Qassim shamkhi

Department of Physics, College of Science, Kufa University
e-mail: qassim-shamkhi@yahoo.com

Abstract

In this paper the ground state for $Na^{9+}, Mg^{10+}, Al^{11+}$ ions has been studied by using Hartree-Fock wave function, the total energy, kinetic energy, potential energy, radial expectation values $\langle r^n \rangle (n = 2,1,0,-1,-2)$, We found the Hartree-Fock ground energy of Na^{9+}= -114.231 hartree, of the Mg^{10+}= -136.605 hartree and E_h of the Al^{11+}= -160.993hartree. the total ground state energy gives results a good agreement with other results published.

Key words: atomic properties , K-Shell , Hartree-Fock

دراســـــــــة الخــواص الذريــــــــة في القشـــرة K للأيونات Al^{11+} , Mg^{10+} , Na^{9+} في فضاء الموقع

انتصار فرحان سلمان   قاسم شمخي جبار

الخلاصة :

في هذا البحث الحالة الارضية للأيونات Al^{11+} , Mg^{10+} , Na^{9+} درست باستخدام الدالة الموجية لهارتري–فوك ، الطاقة الكلية ، الطاقة الحركية ، طاقة الجهد ، والقيم المتوقعة للمسافة بين الالكترون والنواة عند قيم (2,1,0,-1,-2 =n) درست ايضا. حيث وجدنا ان طاقة هارتري-فوك لأيون الصوديوم hartree 114.231 - = Na^{9+} ولأيون المغنسيوم -= Mg^{10+} 136.605H واخيرا كانت طاقة هارتري-فوك لأيون الالمنيوم 160.993H- = Al^{11+} . الطاقة الكلية للحالة الارضية للأيونات اعطت نتائج متوافقة جداً مع نتائج اخرى منشورة .

كلمات مفتاحية: الخواص الذرية ، دالة هارتري- فوك ، الغلاف الذري

1.Introdation:

Two-electron atoms or ions present an excellent testing ground for checking new calculation approaches and for studying photoelectron and other atomic processes. However, the Schrödinger equation for atoms/ions with more one electron cannot be solved analytically. Approximation methods must be applied in order to solve the problem, a large variety of techniques were developed to obtain the non-relativistic bound energies and wave function for mentioned system an excellent review on this topic can be found in[1,2]. In general, a large number of approximation must be introduced to obtained solution. The approximation most widely used in calculating the details of atomic structure is the self-consistent field Hartree-Fock method[3]The Hartree-Fock(HF) approximation ignores the correlation between electrons, but gives roughly 99% of the total electronic energy. Moreover, it is often accurate for the predication of atomic structure. Unfortunately, the part of the energy which the Hartree-Fock approximation ignores can have important chemical effects and this is particularly true when bonds are formed and/or broken. Consequently, realistic model chemistries require a satisfactory treatment of electronic correlation. The concept of electron correlation E_C was introduced by Wigner and defined as[4],

$$E_C = E - E_{HF} \quad …(1)$$

Where E is the exact non-relativistic energy, i.e., the difference between the correlated and the Hartree-Fock energiesE_{HF}, is also shown. In parentheses we give the statistical error in the calculation[5]. In this work we are studied the energy for the He-like ions $(Na^{9+}, Mg^{10+}, Al^{11+})$and compared with the corresponding experimental values.

2. Theoretical Background

The atomic theory is largely based on the independent-electron model which assumes each electron as moving in the combined field of the nucleus and the average distribution of the other electrons. Here the effect of interelectronic repulsion, globally referred to as correlation[6]. Ground state Hartree-Fock(HF) theory not only has proven a valuable tool to calculate the ground state properties of electronic systems, but has also served as a starting point for more sophisticated approaches which deal with correlation, like configuration interaction methods and density functional theory(DFT). Ground state HF theory is based on the Rayleigh-Ritz variational principle, which states that the expectation value of the Hamiltonian *H* of the *N*-electron system(atomic units)[7],

$$H = \sum_i \left[-\frac{\nabla_i^2}{2} + U_{xi}(r_i) + \frac{1}{2}\sum_j^i \frac{1}{|r_i - r_j|} \right] \quad …(2)$$

$\frac{\nabla_i^2}{2}$ kinetic energy, $U_{xi}(r_i)$ attraction term

Attains its minimum value for the true ground state energy E_o:

$$\langle \Psi|H|\Psi \rangle \geq E_o \qquad …(3)$$

Where Ψ is any normalized N-electron antisym- metric state. Let us take $N^\uparrow$ and $N^\downarrow$ to be the number of spin-up and spin-down electrons in the ground state, $N = N^\uparrow + N^\downarrow$. In the (unrestricted) HF approximation, one substitutes a trial N-particle Slater determinant ,

$$\emptyset_o = \frac{1}{\sqrt{N!}} det[\emptyset_1^\uparrow, …, \emptyset_{N^\uparrow}^\uparrow; \emptyset_1^\downarrow, …, \emptyset_{N^\downarrow}^\downarrow] \quad …(4)$$

For Ψ and minimizes the expectation value $\langle \emptyset_o|H|\emptyset_o \rangle$ with respect to the spin orbitals $\emptyset_j^\sigma$ of $\emptyset_o$. The minimization results in single particle Schrödinger-like equations which determine $\emptyset_j^\sigma$:

$$h_{\emptyset_o} \emptyset_j^\sigma(r) = c_j^\sigma \emptyset_j^\sigma(r), \qquad …(5)$$

The spatial part of the atomic orbitals is written in terms of the spherical harmonics[8],

$$\emptyset(r) = R_{nl}(r) Y_{lm_l}(\Omega) \qquad …(6)$$

and the radial atomic number orbitals R_{nl} have been expanded in terms of Slater-type basis function,

$$R_{nl}(r) = \sum_{j=1}^{M} C_{jln} S_{jl}(r) \qquad …(7)$$

where $S_{jl}(r)$ is given by,

$$S_{jl}(r) = N r^l e^{-\xi r} \qquad …(8)$$

and the normalization constant N is,

$$N = \frac{(2\xi)^{n+1/2}}{\sqrt{(2n)!}} \qquad …(9)$$

3. Results and Discussion

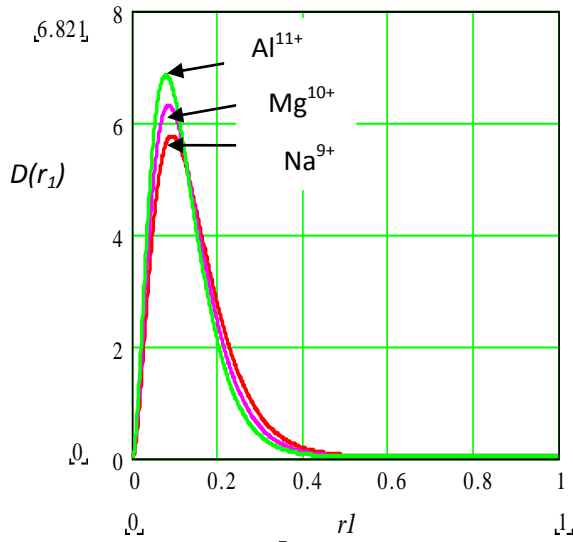In position space, systematic data of the electron-pair were reported in Ref[8],at Hartree-Fock wavefunction for iso-electronic of He atom Clemeti and Roetti using these data, we have calculated the atomic properties for $Na^{9+}, Mg^{10+}, Al^{11+}$ ions.

We calculated the radial density distribution function $D(r_1)$ by using eq(1a) in Ref[9], inter-practical density distribution function $f(r_{12})$ according to eq(3) in Ref[10], The potential and total energies according to eq(23),(24)in Ref[11], the results of all energies are listed in Tables(3) and plotted in Figures(3),(4), Each plot in this work was normalized to unity and all results of the expectation values checked according to the normalization condition. Several attitudes are deduced from Table(2). As the nuclear charge Z increases the expectation values r^n (represent the nuclear-electron distance) increases for all ions. This includes magnitude of the electron density n = -2,-1,1,2. The zero quantity is the normalization integral $\langle r^n \rangle = \int_0^\infty r^n D(r) dr$.

All $<r^2>$ give the diamagnetic susceptibility, $<r^{-1}>$ give the nuclear magnetic shielding constant. Figure[1]demonstrates the probability of finding an electron near nucleus, it increase when the charge nuclear increase of all ions under study.

Table(1): One-particle expectation value for each ions the HF densities were calculated from the wavefunctions of Clementi; atomi units are used through.

ions	$\langle r_1^{-2} \rangle$	$\langle r_1^{-1} \rangle$	$\langle r_1^1 \rangle$	$\langle r_1^2 \rangle$
Na^{+9}	230.224	10.687	0.141	0.027
Mg^{+10}	275.141	11.687	0.129	0.022
Al^{+11}	324.073	12.688	0.119	0.019

Figure(1):   The   radial   density   distribution function as function distance (r_1 a.u).

Table(2):Values of the inter-electron position properties calculated by the Hartree-Fock framework for the ions Na^{9+}, Mg^{10+}, Al^{11+} in *a.u*

ions	$\langle r_{12}^{-2} \rangle$	$\langle r_{12}^{-1} \rangle$	$\langle r_{12}^{1} \rangle$	$\langle r_{12}^{2} \rangle$
Na^{+9}	75.796	6.652	0.206	0.053
Mg^{+10}	90.681	7.278	0.188	0.045
Al^{+11}	106.906	7.903	0.173	0.038

And   when   the   distance   between   nucleus-electron become small, from The figure(1) it can be seen that the probability for Na^{9+} = 5.732 when $r = 0.096$, for Mg^{10+}= 6.2601 when $r = 0.090$, for Al^{11+}= 6.821 when $r = 0.079$. and the for all ions becomes zero when the $r=\infty$.
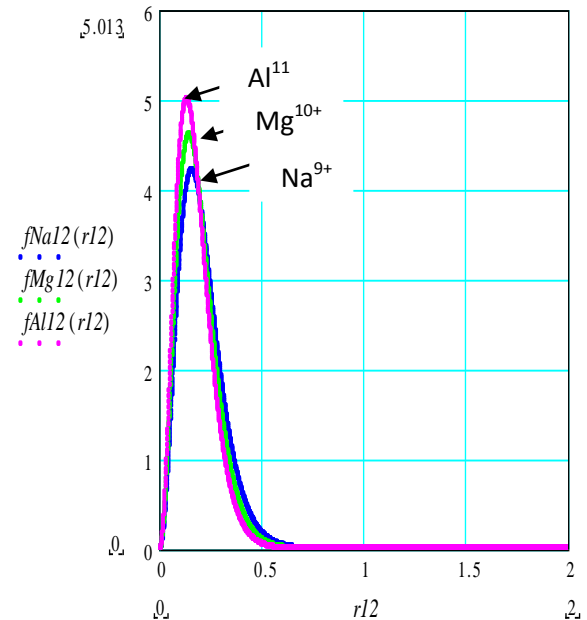
Table(2) give the inter-particle expectation values $\langle r_{12}^{n} \rangle$ $n = -2$ to 2 , were obtained by evaluating

$$\langle r_{12}^{n} \rangle = \int_{0}^{\infty} r_{12}^{n} f(r_{12}) dr_{12}$$

the   distance   between   electron–electron increases for all ions when the nuclear charge increases this means the repulsion between two-electron increases when Z increases. From Figure(2), It can be seen that the maximum value for $f(r_{12})$ for Al^{11+} equal to 5.013 when the distance between electron-electron $r_{12}=$ 0.131 this value more than maximum value $f(r_{12})$ for Na^{9+} = 4.216 when r_{12}= 0.157 a.u, and for Mg^{10+} $f(r_{12})$ =4.6146 when $r_{12} = 0.143$ a.u.


Figure(2): the inter-particle distribution function for He-like ions As function of r_{12}.

The results of the expectation values $<V_{en}>$, $<\cdots>$, $<E_{HF}>$ are listed in table(4), and re $f(r_{12})$ $<V>,<E_{HF}>$ plotted in Figures(3),(4) as   ion Z. The $<V>$, $<E_{HF}>$ exhibit a ge   nd to increase as Z increases in this case of the $<V>$, $<E_{HF}>$,

Table(3): Hartree-Fock energy for the ground state of Na^{+9}, Mg^{+10}, Al^{+11} are listed and comparison, in which E_{HF} were reported in *Ref*[12]. All values are in hartree.

ions	$<V_{en}>$	$<V_{ee}>$	$<V>$	$<E_{HF}>$	*Ref[12]*
Na^{+9}	235.114	6.652	228.462	114.231	114.236
Mg^{+10}	280.488	7.278	273.210	136.605	136.611
Al^{+11}	329.888	7.903	321.985	160.993	160.986

Al^{11+} ion has thoroughly large value than Na^{9+}, Mg^{10+}, We compared this result with *I.Chen et al(2010)* were found large agreement between them.
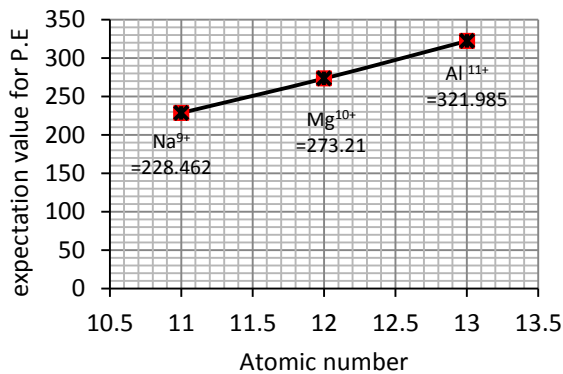
Figure(3): the expectation value for potential energy As a function of atomic number.
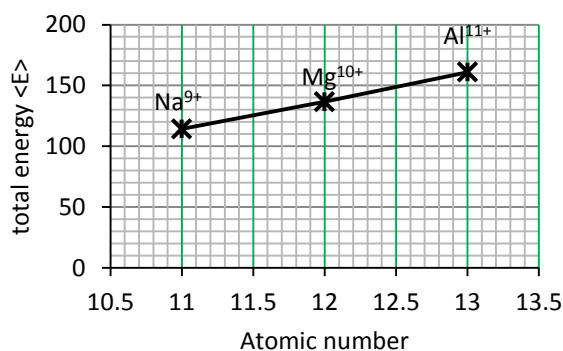
Figure(4): the expectation value for total energy for all ions under studying as a function of atomic number.

Conclusions

We studied the atomic properties for Na^{+9}, Mg^{+10}, Al^{+11} ions in S-state of the two-electron atomic system. All the properties $D(r_1)$, $f(r_{12})$,

$<V_{en}>,<V_{ee}>,<V>,<E_{HF}>$ increases as Z increases.As Z increased the values of $\langle r_1^n \rangle$, $\langle r_{12}^n \rangle$ increases for n negative values and decreased for n positive values.

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