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Expected Values of Electron Potential and Total Energy in Li, Be^{+}, B^{2+} Atomic Structures

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Abstract

The absorption spectra of anthracene were studied and measured in the non-polar solvent cyclohexane and in the polar solvent methanol at two concentrations [10^{-4} M] and [10^{-5} M]. The results showed a small shift of the absorption spectra of anthracene towards longer wavelengths (red shift) in the non-polar solvent (cyclohexane). These measurements were made at room temperature (20°C).

Keywords: Hartree-Fock; Potential energy; Total energy; Single particle; Expected value
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1. Introduction

Fock first introduced the Hartree-Fock (HF) equations in 1930.Since then, research on atomic and molecule electronic structure has relied heavily on the Hartree-Fock technique. The creation of efficient Hartree-Fock equation computing techniques For Hartree-Fock equations, there are two calculation approaches: algebraic and numerical [1]. Numerical computational methods have been developed for atomic HF equations [2,3]. The partitioning technique has been used to evaluate the open shell system of the Be ($1s^2$ $2s^2$) state using the Hartree-Fock wave function as a Slater determinant. We consider six pairs of electronic wave functions for the Be atom, two for intra-shells (K,L) and two for inter-shells (KL). The one-electron expectation value can be calculated for each wave function from the radial electronic density function D(r1) for the Be atom's 2S state [4]. The ground state and each of the various excited states (1s 2ns) and (n = 3, 4, 5) of Li atom and Li-like ions like Be^{1+}, B^{2+}, and C^{3+} are evaluated, along with the potential energy, total energy, one electron expectation value, and inter-electron expectation value (where n is an integer takes the value -2,-1, 1, 2). The distinctions between singlet and triplet states' electronic distributions are systematically studied. [5]. For a range of excited states ($1s^2$ $2s^2$ ns^1) where n equals (3, 4, 5), boron atoms and related ions, such as C^{1+} and N^{2+}, are examined applying the Hartree-Fock approximation [6].

2. Model and Treatment

Utilizing the $D(r_1)$ radial density function for a single particle [7]:

$$D(r_1) = \int_0^{\infty} D(r_1, r_2)\, dr_2 \tag{1}$$

We can calculate the expected value for a single particle as shown in the following equation [7,8]:

$$< r_1^n >= \int_0^{\infty} D(r_1)\, r_1^n\, dr_2 \tag{2}$$

for n: $+2 \geq n \geq -2$

When n=0, the expected value must equal one (standard condition):

$$\int_0^{\infty} D(r_1) r_1^0\, dr_2 = \int_0^{\infty} D(r_1)\, dr_2 = 1 \tag{3}$$

It represents $< r_1^n >$ the maximum probability of finding an electron in certain locations of the nucleus and is related to the radial probability density of the particle.

For the shell K :

$$< r_1^n >= \int_0^{\infty} R_{1S}^2\,(r_1) r_1^2 r_1^n\, dr_1 \tag{4}$$

For the shell L(1S) :

$$< r_1^n >= \int_0^{\infty} R_{2S}^2\,(r_1) r_1^2 r_1^n\, dr_1 \tag{5}$$

Expected value of the distance between two electrons as in the following equation [8,9]:

$$< r_{12}^n >= \int_0^{\infty} f(r_{12})\, r_{12}^n\, dr_{12} \tag{6}$$

The angular distribution function [10]:

$$f(r_{12}) = \begin{bmatrix} 0.5\, r_{12} \int_{r_{12}}^{\infty} r_1 \int_{r_1 - r_{12}}^{r_1 + r_{12}} R^2(r_1)\, R^2(r_2) r_2 dr_2 dr_1 \\ + \int_0^{r_{12}} r_1 \int_{r_{12} - r_1}^{r_{12} + r_1} R^2(r_1)\, R^2(r_2) r_2 dr_2 dr_1 \end{bmatrix} \tag{7}$$

We can also calculate the expected value for the total potential energy [11]:

$$< \mathrm{V} >= -\mathrm{Z} \sum_{\mathrm{i}=1}^{\mathrm{N}} < \mathrm{r}_{\mathrm{i}}^{-1} > + \sum_{\mathrm{i}<j}^{\mathrm{N}} < \mathrm{r}_{\mathrm{ij}}^{-1} >$$

When i=1, j=2:

$$< \mathrm{V} >= -\mathrm{Z} < \mathrm{r}_1^{-1} > + < \mathrm{r}_{12}^{-1} > \tag{8}$$

The expected value for the total potential energy [12]:

$$< E >= \frac{1}{2} < V > \tag{9}$$

3. Results and Discussion

Tables (1) and (2) present the results of the one-particle expectation values for the entire ground state and various excited states of Li-like ions up to Z=5 for varying powers (n=-2 to 2). We observed from these tables the impact of increasing the atomic number while maintaining the same amount of electrons. When (n) assumes negative values, it is seen that the expectation values grow as the atomic number decreases; the values of $\langle r_1^n \rangle$ indicate attractiveness.energy between the electron and the nucleus, but when (n) acquires positive values, the anticipated values of $\langle r_1^n \rangle$ fall because as nuclear charge grows, the distance between the electron and the nucleus gets smaller.For every wave function, a normalizing condition has been implemented.

Table (1) The expected value of one particle of the K shell of the lithium atom and similar ions

Atom or ion	Z	$\langle r_1^n \rangle$				
		n=-2	n=-1	n=0	n=1	n=2
Li	3	14.88829	2.68503	1	0.57312	0.44680
Be$^+$	4	27.76744	3.68244	1	0.41498	0.23303
B^{+2}	5	44.64037	4.68068	1	0.32521	0.14268

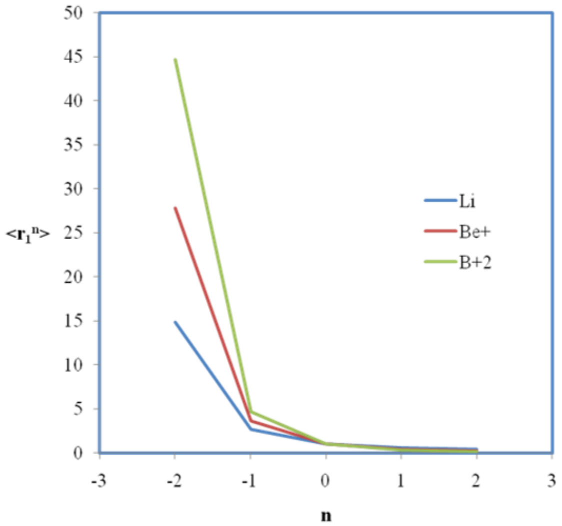

Fig. (1) Determining the value of one particle of the K shell for the lithium atom and similar ions

Table (2) Expected value of one particle of the L shell of the lithium atom and similar ions

Atom or ion	Z	$\langle r_1^n \rangle$				
		n=-2	n=-1	n=0	n=1	n=2
Li	3	0.43542	0.34539	1	3.87365	17.78413
Be$^+$	4	1.45097	0.60746	1	2.28009	6.08913
B^{+2}	5	2.98472	0.86335	1	1.63630	3.12874

The inter-particle expectation value results are shown in table (3). We observed that when (n) takes negative values, $\langle r_{12}^n \rangle$, the expectation values increase as the atomic number increases for all different configuration states, where the repulsion energy between two electrons is represented by the value $\langle r_{12}^{-1} \rangle$, and when (n) takes positive values, $\langle r_{12}^n \rangle$ decreases.

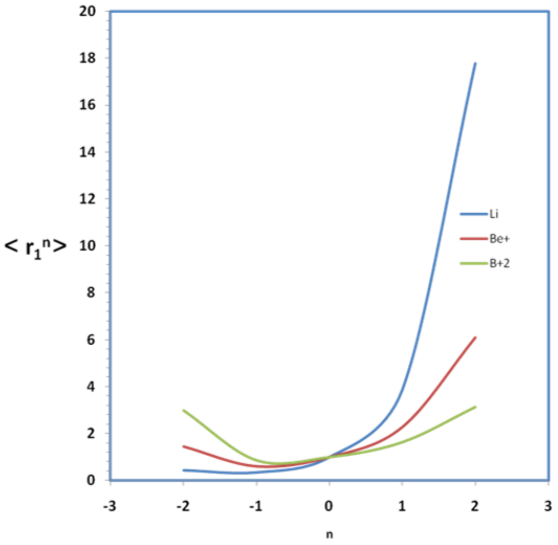

Fig. (2) Expected value of one particle of the L shell of the lithium atom and similar ions

Table (3) The expected value of the inter-shell distance K for the lithium atom and similar ions

Atom or ion	Z	$\langle r_{12}^n \rangle$				
		n=-2	n=-1	n=0	n=1	n=2
Li	3	4.71722	1.64988	1	0.83950	0.89360
Be$^+$	4	8.91738	2.27322	1	0.60714	0.46607
B^{+2}	5	14.44859	2.89708	1	0.47549	0.28536

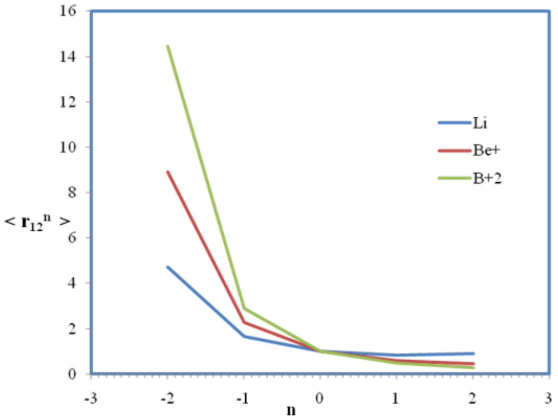

Fig. (3) The expected value of the inter-shell distance K for the lithium atom and similar ions

The expected values for the potential energy and total energy of the system under study are shown in table (4). Based on these findings, we saw that all energies increased as the atomic number increased, as a result of rising (Z).

Table (4) The expected value of the potential and total energy of a Li atom and similar ions

Atom or ion	*Z*	*Shell*	⟨*V*⟩	⟨*E*⟩
Li	3	*K* *L* *Total*	-14.460309 -1.036174	-7.23015427986 -0.5180869723 -7.42557636 -7.432726924 [13]
Be$^+$	4	*K* *L* *Total*	-27.186365 -2.429866	-13.59318248925 -1.2149329994 -14.25965119 -14.27739 [14]
B^{+2}	5	*K* *L* *Total*	-43.909742 -4.316796	-21.95487089776 -2.158398246 -23.34760385 -23.37598 [14]

4. Conclusion

The expected value of the probability of finding an electron around the nucleus is equal to one when n=0, and this is the standard condition. With the increase in the atomic number, the expected value of the probability of the presence of electrons around the nucleus increases at negative values of n, i.e. in areas close to the nucleus due to the force of attraction between the nucleus and the electrons, and the expected value of the probability of the presence of electrons around the nucleus decreases at positive values of n due to the weakness of the force of attraction between the nucleus and the electrons. The expected values of potential and total energy increase with increasing atomic number. The expected value of the total potential energy in the K shell is greater than in the L shell. This is because the electrons in the K shell are close to the nucleus, and the electrons are as close as possible to each other. If we move to the L shell, the electrons will move away from the nucleus and the distance between them will increase, in addition to the presence of electron shielding in the K orbital.

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