Studies on Nuclear Magnetic Shielding Constants for Isoelectronic Series of the Atoms He, Li, and Be Using Improved Roothan-Hartree-Fock Wave-Functions

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Abstract

A simple theoretical approach is developed to calculate the nuclear magnetic shielding (*NMS*) constant σ for atoms *He*, *Li*, *Be* and their isoelectronic series using Roothan-Hartree-Fock (*RHF*) wave functions which were improved by Koga, et al (*1995*).The calculations carried out have been extended to the intra- and inter-shells (singlet and triplet states) of atoms and ions to calculate σ for $K_\alpha K_\beta$, $K_\alpha L_\alpha$, and $L_\alpha L_\beta$, to find the contribution from these correlated states to the *NMS* constant σ. In order to calculate the nuclear magnetic shielding constant, the theoretical relations such as the one particle radial density distribution function *D(r)* and one particle expectation value $\langle 1/r \rangle$ for all states have been derived analytically and programmed in MATHCAD program .The results obtained which are given in tables and in graphical plots are interpreted and discussed in some details. The reliability of the approach is verified by comparing our results with those previously reported.

Key wards: *Nuclear magnetic shielding constant σ, Intra- and inter-electronic shells NMS constant, Roothan-Hartree-Fock wave functions.*

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1. Introduction

The determination of nuclear magnetic shielding *(NMS)* constant σ with high precision remains an important area of study. *NMS* constant plays an important part in studying the nuclear magnetic resonance *(NMR)* spectroscopy. *NMR* spectroscopy in solutions for example is a widely used as a tool for studying the structure and dynamics of materials in areas of chemistry, biology, and medicine. In addition, for spherically symmetric approximations the *NMS* constant σ is related to the coherent X-ray scattering amplitude, which opens up an experimental route to *NMS* constant σ [1].

Since the work of Hylleraas on the calculation of the nuclear magnetic shielding constant σ for *He* and H_2 [2], there has been numerous modeling works done based on Hartree-Fock wave functions [3,4]. The *NMS* constant for atoms and molecules has been also investigated experimentally by many authors [5-7].

Although several studies are published yearly on the calculation of nuclear magnetic shielding constant σ for some atoms and ions, little quantitative information is available on the elementary contribution from the intra- and inter-electronic shells in atomic and ionic orbitals in some details. However, to our knowledge, the literature contains no specific studies to the nuclear magnetic shielding constant of the intra- and inter-electronic shells, and their contributions to *NMS* constant σ. This is primarily due to the difficulty in solving the mathematical problems. Moreover, the physical constants required for these studies, are often only known with moderate accuracy. Electron correlation effects in Li-like ions have been examined in some detail for intra-and inter-shells [8].

The main aim of the present work is devoted to studing certain points concerning calculation of nuclear magnetic shielding constant σ. We report explicit formulae and response calculations for the special case of closed-shell atoms, the noble gas *He* and *He-like* ions, the alkali metal *Li* with unpaired electron in the $2S$ state and *Li-like* ions as well, and finally the *Be* atom with two electrons in the $2S$ state, and its isoelectronic sequence. The determination of the expectation value $\langle\frac{1}{r}\rangle$ requires the evaluation of electron radial density distribution function *D(r)*. From $<1/r>$ we determined the NMS constant σ.

To see the influence of the unpaired electron in the $2S$ state for *Li-like* ions on the *NMS* constant σ, we have calculated the *NMS* constant for the $K_\alpha K_\beta$, and $K_\alpha L_\alpha$. In the case of *Be-like* ions we have calculated the *NMS* constant for the $K_\alpha K_\beta$, $K_\alpha L_\alpha$, and $L_\alpha L_\beta$. These contributions from the external orbit as compared to the inner one have not received a theoretical foundation[9]. We have used in our calculations *RHF* wave functions with optimized orbital exponents which have been improved by Koga et al [10] in 1995.

2. Theoretical background:

2.1 Nuclear Magnetic Shielding Constant Calculations:

For ^1S states of one-electron atom and ions the *NMS* constant σ is given by Hylleraas and Skavlem [2] as:

$$\sigma = \frac{1}{3}\alpha^2\langle\frac{a_H}{r}\rangle \qquad (1)$$

Where a_H is the Bohr radius, α is the fine structure constant, and r is the distance from the nucleus to electron.

While for ^1S states of n-electron atoms and ions, the *NMS* constant σ could be written in the form:

$$\sigma = \frac{1}{3}\alpha^2 \sum_{i=1}^{n} \langle \frac{a_H}{r_i} \rangle \tag{2}$$

The expectation value is written as: $\langle a_H / r \rangle = \int \psi^* \frac{a_H}{r} \psi \, d\tau$ and the *NMS* constant σ takes the form:

$$\sigma = (\frac{\alpha^2}{3}) \int \psi^* \left[\sum_{i=1}^{n} \frac{a_H}{r_i} \right] \psi . d\tau \tag{3}$$

Where ψ represents the HF wave function.

2.2 HF wave function approximation

The Hartree-Fock (*HF*) atomic wave functions are independent particle model approximations to non relativistic Schrödenger equation for stationary states. In conventional (*HF*) approximation, the orbitals spin are expressed as products of a radial function times a spherical harmonic times a spin function. Roothaan- Hartree-Fock (*RHF*) or analytic self consistent–field (*SCF*) the atomic wave functions are approximations to conventional HF wave functions in which the radial atomic orbitals are expanded as a finite superposition of primitive radial functions[11]. Koga et al in (1995) improved (*RHF*) wave functions for isoelectronic series of the atoms He to Ne which yield lower energies than those of Clementi and Roetti[10]. The HF wave function for n-electron atoms and ions is defined as single Slater determinant as:

$$\psi_{HF} = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(1)\alpha(1)\varphi_2(1)\alpha(1)\ldots\ldots\varphi_N(1)\beta(1) \\ \varphi_1(2)\alpha(2)\varphi_2(2)\alpha(2)\ldots\ldots\varphi_N(2)\beta(2) \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ \varphi_1(N)\alpha(N)\varphi_2(N)\ldots\ldots\varphi_N(N)\beta(N) \end{vmatrix} \tag{4}$$

α and β refer to the two components of the spin part (up & down). The orbitals, in turn, are written as an expansion in some set of analytic basis functions as[12]:

$$\varphi_{nl} = \sum_{i=1}^{N} C_n^i \chi_{nlm_l}^i \tag{5}$$

The factors C_n^i are taken to minimize the total energy and the basis function χ_{nlm_l} is the standard Slater-type orbitals and is given by:

$$\chi_{nlm_l}(r,\theta,\varphi) = R_{nl}(r) Y_{lm_l}(\theta,\varphi) \tag{6}$$

Where

$$R_{nl}(r) = N_{nlm_l} r^{n-1} e^{-\xi r} \tag{7}$$

Where ζ the orbital exponent constant is used to optimize RHF wave function, $R_{nl}(r)$ represents the redial part of the wave function which is equal to φ_{nl} after integrating over the angular part, so it is given by:

$$R_{nl} = C_n N_{nlm} S_{nl}(r) \tag{8}$$

N_{nlm} is the normalization constant, it is given by :

$$N_{nlm} = \frac{(2\zeta)^{n+\frac{1}{2}}}{[(2n)!]^{\frac{1}{2}}} \tag{9}$$

Where $S_{nl}(r)$ is called Slater type orbitals (STO's) defined by

$$S_{nl}(r) = r^{n-1} e^{-\zeta r} \tag{10}$$

And $Y_{lm}((\theta,\varphi)$ is the angular part of the wave function.

2.3 The radial density distribution function D(r)

The electronic density function can be regarded as the central quantity for the evaluation of nondifferential one electron properties[13].The one-particle radial density distribution function $D(r)$, is very important in the study of the electrons in an atom, it is defined as a measure of the probability of finding the electron in each shell such as that, its radial coordinate is in the range of r to $r+dr$. Or, in other words it represents the density distribution of one electron in each shell.

The radial electronic density distribution function $D(r)$ is evaluated from the two-particle radial density distribution $D(r_1, r_2)$ as:

$$D(r_1) = \int D(r_1, r_2) r_1^2 r_2^2 dr_2 \tag{11}$$

Where:

$$D(r_1, r_2) = N \iint \psi^*(1,2)\psi(1,2) r_1^2 r_2^2 d\Omega_1 d\Omega_2 \tag{12}$$

With $d\Omega_i = \sin\theta_i d\theta_i d\varphi_i$ and $i = 1$ or 2 such that $\int_0^\infty \int_0^\infty D(r_1, r_2) dr_1 dr_2 = 2$.

2.3.1 He-like ions

The calculation of *NMS* constant σ for an atom or ion with closed electronic shells is easy in principle. If one knows the atomic or ionic wave function to some degree of accuracy, the rest of the work is to sum up the mean reciprocal values of the electronic distances from nuclei.

For two electron atoms or ions (K-shell), the radial electron distribution function is found to be of the form:

$$D(r)) = R_{1s}^2(r)r^2 \tag{13}$$

2.3.2 Li-like ions

For ^2S states, the unpaired electron spin magnetic moment interacts with both the nuclear magnetic moment and the external magnetic field. The behavior of a nucleus having a nonzero magnetic moment in an external magnetic field is further complicated compared with those of closed electronic shells. For three-electron atoms or ions the radial density distribution for both $K_\alpha L_\alpha (= K_\beta L_\alpha)$ is of the form:

$$D(r) = \frac{1}{2}[R_{1s}(r) + R_{2s}(r)]^2 r^2 \tag{14}$$

2.3.3 Be-like ions

In this case we have ^2S states, but with one pair of electrons, then the electron radial density distribution for singlet and triplet states could be written respectively as:

$$D(r) = \frac{1}{2}\left[R_{1s}^2(r) + R_{2s}^2(r) + 2R_{1s}(r)R_{2s}(r)\right]r^2 \tag{15}$$

And

$$D(r) = \frac{1}{2}\left[R_{1s}^2(r) + R_{2s}^2(r) - 2R_{1s}(r)R_{2s}(r)\right]r^2 \tag{16}$$

2.4 Determination of the expectation values

The expectation value $\langle 1/r \rangle$ for the above mentioned series is determined from the expression[14]

$$\langle r^n \rangle = \int_0^\infty D(r) r^n dr \tag{17}$$

The case $n = -1$ leads to the electron-nuclear potential energy and the NMS; $n = 2$ is required to evaluate the diamagnetic susceptibility, and some of the moments can be related to various oscillator strength sums [1]. By direct substitution for *D(r)* from equations (13), (14), (15), and (16) into equation (17) and integrating, the expectation value $\langle 1/r \rangle$ has been obtained for *He*-, *Li*-, and *Be*-like ions.

The computed values of *NMS* constant σ and the expectation values $\langle 1/r \rangle$ are summarized in tables 1-5.Tables 1, 2, and 4 also report the value $\Delta\sigma$ which is defined as the difference in NMS constant σ between two successive ions in each isoelectronic series as:

$$\Delta\sigma = \sigma\left(X^{(n+1)+}\right) - \sigma\left(X^{n+}\right) \tag{18}$$

With $n = 0,1,2,3,\ldots$, up to the end of the sequence.

Table 1 *NMS* constant σ and the expectation value $\langle 1/r \rangle$ for He-like ions from Z = 2-11.

System	NMS constant σ $\times 10^{-5}$	$\Delta\sigma$	$\langle 1/r \rangle$
He	5.99000	3.55058	1.68728
Li^{+}	9.54058	3.55022	2.68742
Be^{2+}	13.0908	3.5502	3.68746
B^{3+}	16.6410	3.5501	4.68747
C^{4+}	20.1911	3.5501	5.68748
N^{5+}	23.7412	3.5501	6.68749
O^{6+}	27.2913	3.5501	7.68749
F^{7+}	30.8414	3.5501	8.68749
Ne^{8+}	34.3915	3.5501	9.68749
Na^{9+}	37.9416	Average = 3.550177778	10.68749

Table 2 total *NMS* constant σ and σ for $K_\alpha K_\beta$ and $K_\alpha L_\alpha$ shells for Li-like ions from Z = 3-12.

System	NMS constant $\sigma \times 10^{-5}$					
	$K_\alpha K_\beta$	$\Delta\sigma$	$K_\alpha L_\alpha = K_\beta L_\alpha$	$\Delta\sigma$	Total σ	$\Delta\sigma$ Total
Li	9.53211	3.54089	5.37914	2.23561	10.1452	4.0061
Be^{+}	13.073	3.5436	7.61475	2.22597	14.1513	3.9977
B^{2+}	16.6166	3.5454	9.84072	2.24928	18.149	4.022
C^{3+}	20.162	3.5466	12.0900	2.1951	22.171	3.9684
N^{4+}	23.7086	3.5474	14.2851	2.2207	26.1394	3.9944
O^{5+}	27.256	3.5481	16.5058	2.2201	30.1338	3.9942
F^{6+}	30.8041	3.5484	18.7259	2.2199	34.128	3.9941
Ne^{7+}	34.3525	3.5487	20.9458	2.2197	38.1221	3.994
Na^{8+}	37.9012	3.5489	23.1655	2.2195	42.1161	3.994
Mg^{9+}	41.4501	Ave. 3.546443	25.385	Average 2.22228	46.1101	Average 3.99609

Table 3 the expectation value $\langle 1/r \rangle$ within $K_\alpha K_\beta$ and $K_\alpha L_\alpha$ shells for Li-like ions from Z = 3-12.

System	$\langle 1/r \rangle$	
	$K_\alpha K_\beta$	$K_\alpha L_\alpha$
Li	2.68503	1.51521
Be^{+}	3.68245	2.14494
B^{2+}	4.6806	2.77196
C^{3+}	5.67928	3.40555
N^{4+}	6.67831	4.02386
O^{5+}	7.67756	4.64939
F^{6+}	8.67698	5.27478
Ne^{7+}	9.67651	5.90009
Na^{8+}	10.6761	6.52533
Mg^{9+}	11.6758	7.15053

Table 4 *NMS* constant σ within the $K_\alpha K_\beta$, $K_\alpha L_\alpha$, and $L_\alpha L_\beta$ shells for Be-like ions from Z = 4-13.

System	NMS constant $\sigma \times 10^{-5}$							
	$K_\alpha K_\beta$	$\Delta\sigma$	$K_\alpha L_\alpha = K_\beta L_\alpha$	$\Delta\sigma$	$L_\alpha L_\beta$	$\Delta\sigma$	σ Total	$\Delta\sigma$ Total
Be	13.071	3.5405	7.463	2.2275	1.855	0.9146	14.926	4.4551
B^{+}	16.6115	3.5431	9.69055	2.2223	2.7696	0.90165	19.381	4.4448
C^{2+}	20.1546	3.5449	11.9129	2.2207	3.76126	0.89634	23.8259	4.4413
N^{3+}	23.6995	3.5462	14.1336	2.2198	4.5676	0.89361	28.2672	4.4397
O^{4+}	27.2457	3.5469	16.3534	2.2195	5.46121	0.89198	32.7069	4.4389
F^{5+}	30.7926	3.5476	18.5729	2.2193	6.35319	0.89081	37.1458	4.4385
Ne^{6+}	34.3402	3.458	20.7922	2.2191	7.244	0.89037	41.5843	4.4383
Na^{7+}	37.8882	3.5484	23.0113	2.219	8.13437	0.88973	46.0226	4.4381
Mg^{8+}	41.4366	3.5486	25.2303	2.219	9.0241	0.88935	50.4607	4.4375
Al^{9+}	44.9852	Ave. 3.54602	27.4493	Ave. 2.2207	9.91345	Ave. 0.895382	54.8986	Average 4.4414

Table 5 The expectation value $\langle 1/r \rangle$ within the $K_\alpha K_\beta$, $K_\alpha L_\alpha$, and $L_\alpha L_\beta$ shells for Be-like ions from Z = 4-13.

System	$\langle \frac{1}{r} \rangle$		
	$K_\alpha K_\beta$	$K_\alpha L_\alpha = K_\beta L_\alpha$	$L_\alpha L_\beta$
Be	3.68188	2.1022	0.52252
B^+	4.67917	2.72966	0.78015
C^{++}	5.67722	3.35567	1.03413
N^{3+}	6.67576	3.98119	1.28662
O^{4+}	7.67464	4.60649	1.53833
F^{5+}	8.67376	5.23167	1.78959
Ne^{6+}	9.67305	5.8568	2.04055
Na^{7+}	10.67246	6.48189	2.29131
Mg^{8+}	11.67197	7.10695	2.54194
Al^{9+}	12.67155	7.7320	2.79245

3. Results and discussion

The analytical values of the calculated NMS constant σ and the expectation values $< 1/r >$ are given in graphical form as a function of the main parameter, the atomic number Z. Fig. 1 shows the variation of σ and $< 1/r >$ for He-like ions, for $2 \leq Z \leq 11$. As can be seen the regular trends with Z are nicely reproduced. Our calculated values of σ for total and states using improved *RHF* wave function are in good agreement with the high precision non relativistic calculations of King [1]. In order to support our results we calculated the total values as a summation of contribution of intra and inter electronic shells as:

$$\sigma_{tot.} = \frac{1}{2}[\sigma_{K_\alpha K_\beta} + \sigma_{K_\beta L_\alpha} + \sigma_{K_\alpha L_\alpha} + \sigma_{L_\alpha L_\beta}] \qquad (19)$$

Where the factor $\frac{1}{2}$ is the normalization constant. This leads us to suggest that the present values of intra and inter electronic shells are very accurate because the total values of σ are in agreement with those previously reported, for example our result of NMS for Be^+ ion is $14.1513\text{x}10^{-5}$ and the result for King[15] is $14.15401\text{x}10^{-5}$.

It is important to indicate that relativistic corrections for σ are generally observed to be small for light atoms [1], which means, for intermediate and heavy atoms, the relativistic correction to σ should be taken into account.

The expectation value $< 1/r >$ is also a linearly increasing function of Z as shown in Fig 1. It is the component used to determine the energy. Information necessary for the calculation of $< 1/r >$ has been determined which yield precise and well converged values of *NMS* constant σ.

From table 1, we also observe that the value $\Delta\sigma$ is constant with Z to seventh significant figure except when $n = 0$, i.e. for $\Delta\sigma = \sigma(Li^{+}) - \sigma(He)$. The behavior of $\Delta\sigma$ is shown in Fig.2 as a function of Z. Fig.2 suggests that such a relation holds roughly between $\Delta\sigma$ and small Z ($Z < 5$).

But for ($Z \geq 3$) the relation holds with an average constant $(\Delta\sigma)_{Average}$ equal to $3.550177778 \times 10^{-5}$.

Consequently, we have investigated a simple relation for He-like ions, accurate enough to the point that the results could serve as a calibration guide for the estimation of the value of the *NMS* constant σ as:

$$\sigma\left(X^{(n+1)+}\right) = \sigma\left(X^{n+}\right) + 3.550178 \times 10^{-5}$$

3.1. Influence of the intra and inter-shells

NMS constant σ has been examined in details within the $K_\alpha K_\beta$, $K_\alpha L_\alpha$ shells for the series of Li-like systems with unpaired electron in the ^2S states. For Be-like ions with one pair of electrons in the ^2S states, which are already separated into distinct inner and outer shells, σ has been examined for $K_\alpha K_\beta$, $K_\alpha L_\alpha$ and $L_\alpha L_\beta$ shells. This distinction does not arise for He-series, with only one pair of electrons in the ^1S states.

Fig. 3 shows the analytical values of *NMS* constant σ for several Li-like ions. Also σ for $K_\alpha K_\beta$, and $K_\alpha L_\alpha$ are given in order to find the influence of both shells to the total nuclear magnetic shielding constant σ. The contribution from $K_\alpha L_\alpha$ $(= K_\beta L_\alpha)$ is less effective than from $K_\alpha K_\beta$. The main reason is that, the Coulomb holes for both inter-shells $K_\alpha L_\alpha$ $(= K_\beta L_\alpha)$ are negative at low Z [8]. Hence, the nuclear shielding provided by the inner-shell electron will be reduced.

It is important to point out that the final shielding constant is not simply the sum of both contributions, when the separate contributions $K_\alpha K_\beta$, and $K_\alpha L_\alpha$ are examined. For $Z \leq 3$, the *NMS* constant for $K_\alpha K_\beta$ seems to coincide with total NMS constant σ. But for $Z > 3$ the divergence starts to occur as may be seen from Fig.3.

A high degree of similarity is shown for several Be-like ions as depicted in Fig 6. In addition to $K_\alpha K_\beta$, and $K_\alpha L_\alpha$, we have presented σ for $L_\alpha L_\beta$ as well. For Be-like ions the magnitudes of σ are ordered as $K_\alpha K_\beta > K_\alpha L_\alpha (= K_\beta L_\alpha) > L_\alpha L_\beta$. This suggests the relative importance of the nuclear shielding from the *K*- shells compared to *L*-shells.

The expectation values $< 1/r >$ are given in figures 4 and 7 for several *Li*- and *Be*- like ions respectively, in which the smooth behavior of $< 1/r >$ is shown as a function of Z. From $< 1/r >$ we computed the fairly precise and well converged values for NMS constant σ for $K_\alpha K_\beta$, $K_\alpha L_\alpha$ and $L_\alpha L_\beta$ as well.

Finally, discussion of the Z dependence of the factor $\Delta\sigma$ defined by equation (18) for $K_\alpha K_\beta$, $K_\alpha L_\alpha$ $\left(= K_\beta L_\alpha\right)$ shells of Li-like ions and $K_\alpha K_\beta$, $K_\alpha L_\alpha$ $\left(= K_\beta L_\alpha\right)$ and $L_\alpha L_\beta$ shells for Be-like ions are given in figures 5 and 8 respectively. These two figures indicate that, for the same scale, the similarity is remarkable. Clearly, $\Delta\sigma$ is constant with increasing Z. For a given intra and inter-shells, a comparison again indicates a high degree of similarity among $\Delta\sigma$ characteristics. However differences in details do occur when $Z \leq 5$ for both intra-and inter-shells for each diagram as in the case of He-like ions, discussed earlier in Fig.2. We may summarize our results in the following equation:

$$\sigma\left(X^{(n+1)+}\right) = \sigma\left(X^{n+}\right) + \left(\Delta\sigma\right)_{Average}$$

Where $n = 0,1,2,3,\ldots$ up to the end of the isoelectronic sequence, and $\left(\Delta\sigma\right)_{Average}$ is given in the following table:

System	$\left(\Delta\sigma\right)_{Average}$
He-like ions	3.550178x10^{-5}
Li-like ions $K_\alpha K_\beta$ $K_\alpha L_\alpha = K_\beta L_\alpha$	3.99609x10^{-5} 3.546443x10^{-5} 2.22228x10^{-5}
Be-like ions $K_\alpha K_\beta$ $K_\alpha L_\alpha = K_\beta L_\alpha$ $L_\alpha L_\beta$	4.4414x10^{-5} 3.54602x10^{-5} 2.2207x10^{-5} 0.895382x10^{-5}

4. Conclusion

A reliable theoretical approach was developed to calculate the nuclear magnetic shielding constant σ for *He*-like ions, for $2 \leq Z \leq 11$, Li-like ions, for $3 \leq Z \leq 12$, and Be-like ions, for $4 \leq Z \leq 13$.

The calculations have been carried out using Roothan-Hartree-Fock (*RHF*) wave functions. These wave functions which were improved by Koga et al (1995) still rate among the best, since, these wave functions are useful in studies of isoelectronic sequences where continuity and smoothness in the quality are essential.

The computations have been extended to the intra $K_\alpha K_\beta$ and inter $K_\alpha L_\alpha$ shells for Li-like ions. For Be-like sequence, in addition to $K_\alpha K_\beta$ and $K_\alpha L_\alpha$, we have calculated σ for $L_\alpha L_\beta$ shell. The one electronic density distribution function D(r) has been calculated from the expectation values $\langle 1/r \rangle$ which are presented in tables and in graphical forms in order to calculate the *NMS* constant σ.

The calculations of the nuclear magnetic shielding constants for He-like ions with closed electronic shells are relatively easy in principle. If the atomic wave function is known to some degree of accuracy, one may sum up the mean reciprocal values of the electronic distances from nuclei $\langle 1/r \rangle$ to get σ.

We have calculated also the factor $\Delta\sigma$ defined by eq. (18) for each shell as given in tables 1, 2, and 4. Because of its importance in estimating the *NMS* constant σ for each sequence, this factor is also displayed graphically in figures 2, 5, and 8.

On the other hand, we extended the analysis to a series of open-shell systems by considering several Li-like ions. These three-electron systems, with unpaired electrons in the $2S$ state, represent the simplest examples in which intra- and inter-electronic shells are all present. The nuclear magnetic shielding constant σ of such a nucleus can still be calculated using the most important terms of the developed open-configuration Roothaan-Hartree-Fock wave function which were improved by Koga et al. It was found that the contribution from $K_\alpha K_\beta$ is much greater than that from the $K_\alpha L_\alpha$ inter-shell. This behavior is observed for other isoelectronic sequences such as Be-like ions.

Finally, for Be-like ions with a pair of electrons in the $2S$ state, the similarity is remarkable. The contribution of the most inner-electrons $K_\alpha K_\beta$ is much stronger than the contribution from $K_\alpha L_\alpha$, and $L_\alpha L_\beta$ to the total NMS constant σ due to the high density near the nucleus.

It should be clear that our theoretical treatment of the NMS constant σ is accurate enough to the point that the results obtained could serve as a calibration guide for experimental work. Or we may conclude that the present model offers an avenue to provide a reasonable estimation of the NMS constant σ for atoms and ions.

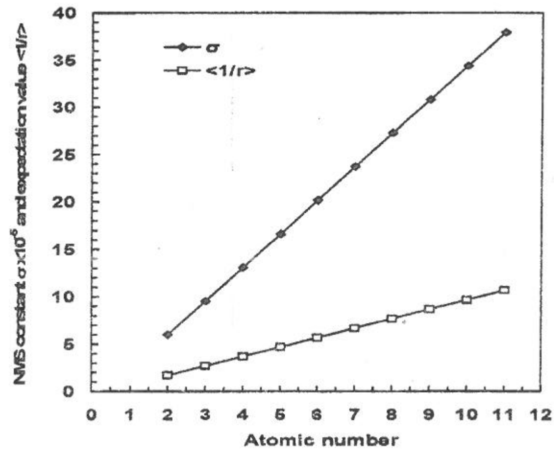

Fig1 NMS constant σ and expectation value <1/r> for He-like ions as a function of atomic number Z

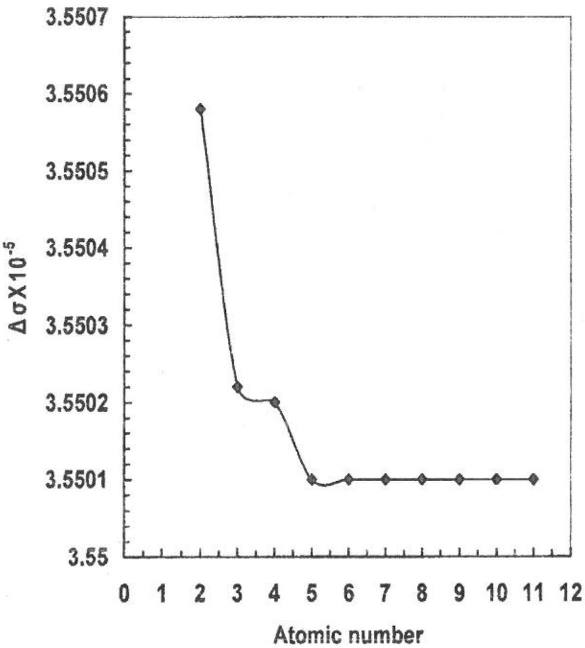

Fig 2. Δσ as a function of atomic number Z for He-like ions

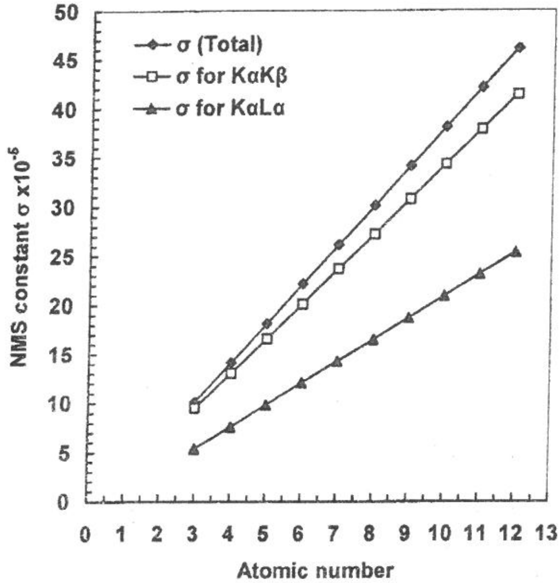

Fig 3 Total NMS constant σ and those for shells $K_\alpha K_\beta$ and $K_\alpha L_\alpha$ for Li-like ions

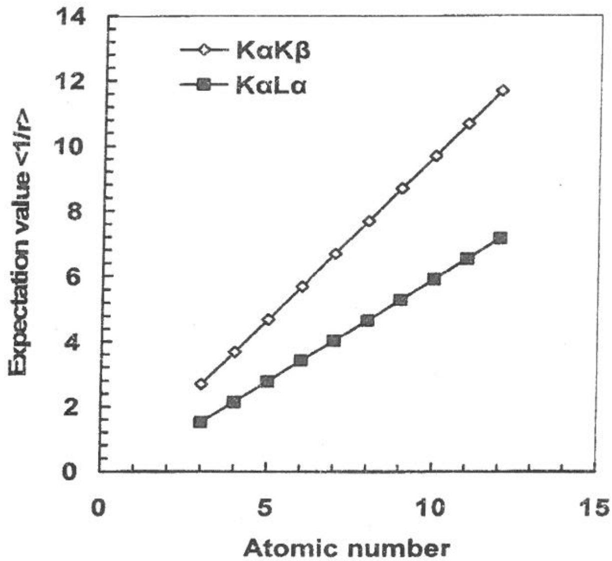

Fig 4 Expectation value <1/r> for Li-like ions as a function of atomic number

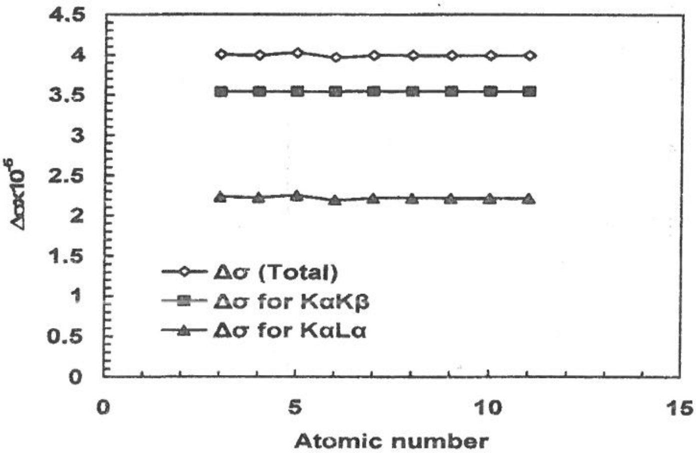

Fig 5 Δσ for Li-like ions as a function of atomic number

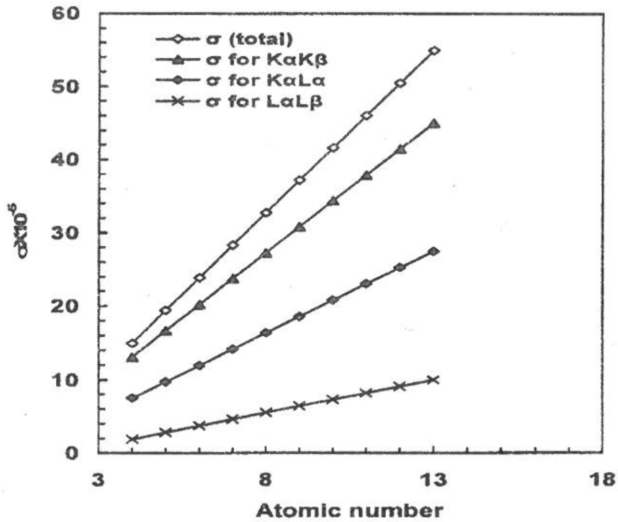

Fig 6 NMS constant for Be-like ions as a function of atomic number Z

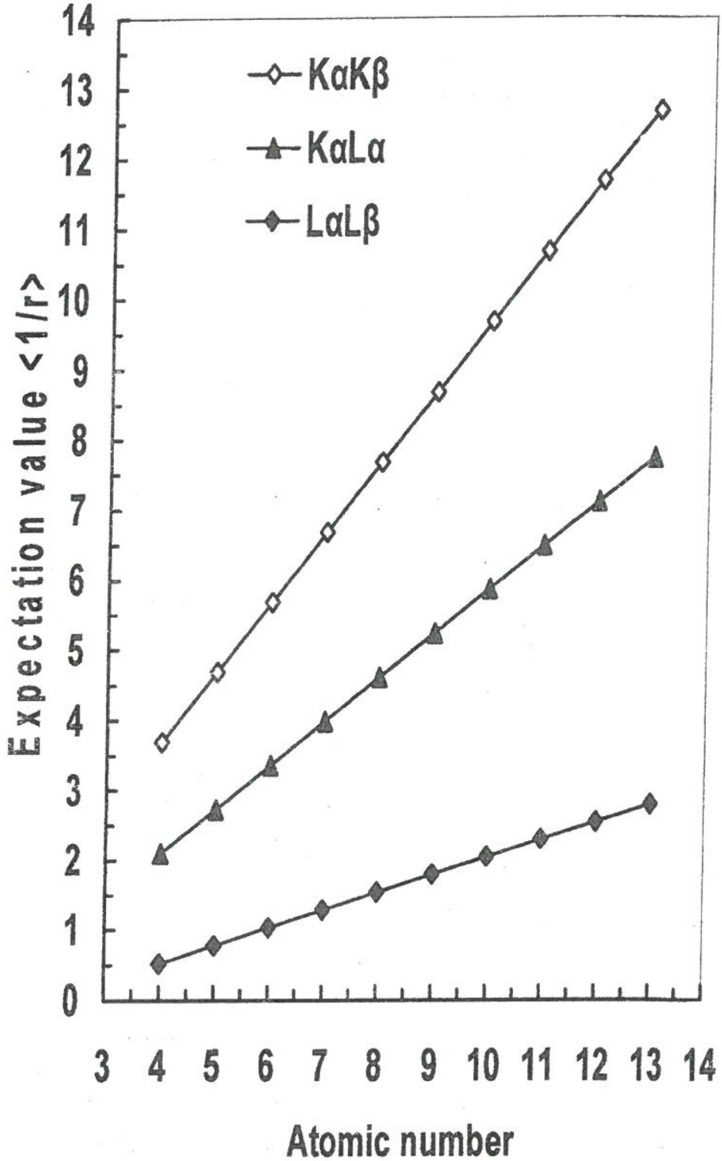

Fig7 Expectation value <1/r> for Be-like ions as a function of atomic number Z

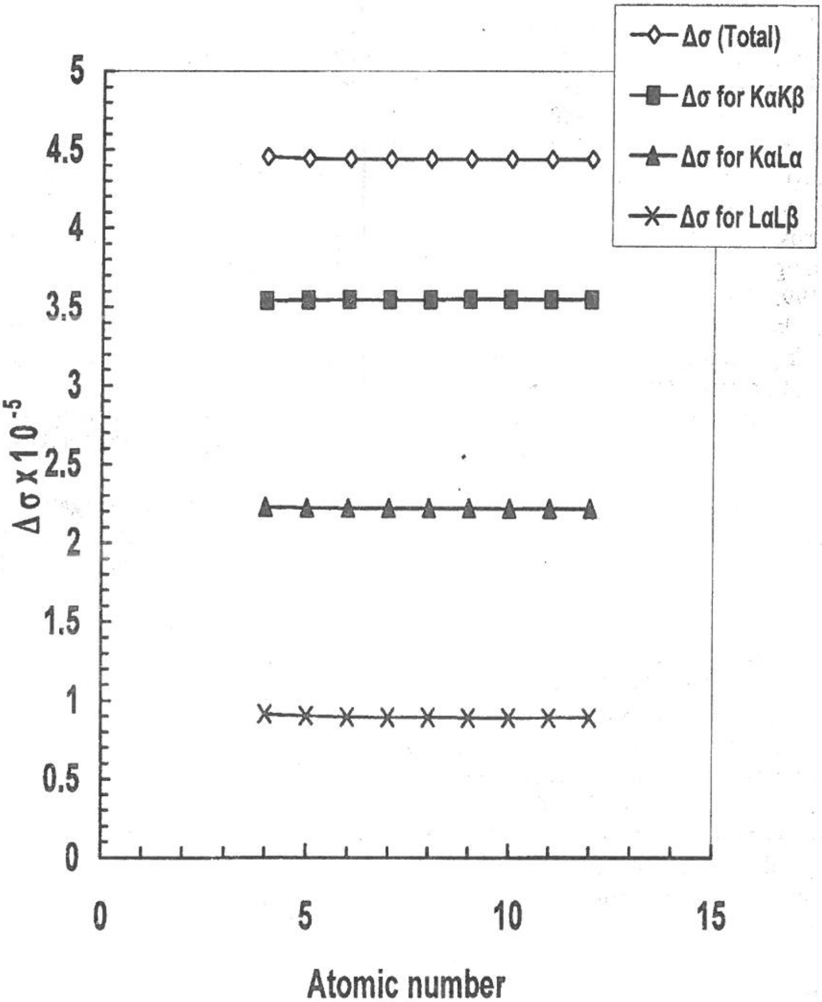

Fig 8 Δσ for Be-like ions as a function of atomic number

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دراسات في ثابت الحجب النووي المغناطيسي للسلاسل المشابهة الكترونيا لذرات He ,Li and Be باستخدام الدوال الموجية لروثان – هارتري – فوك المحسنة .

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الملخص

تم تطوير تقريب نظري مبسط لحساب ثابت الحجب النووي المغناطيسي σ للذرات He ,Li and Be وسلاسلها المشابهة لها الكترونيا باستخدام دوال روثان- هارتري- فوك والتي تم تطويرها من قبل كنج وآخرون (١٩٩٥) . ولقد امتدت الحسابات المنجزة الى حساب ثابت الحجب للحالات الفردية والثلاثية للذرات والايونات قيد الدراسة($K_\alpha K_\beta$, $K_\alpha L_\alpha$ and $L_\alpha L_\beta$) وذلك بهدف تحديد مساهمة هذه الحالات المرتبطة في ثابت الحجب الكلي للذرة. لاجل حساب ثابت الحجب تم اشتقاق علاقتين نظريتين وهما دالةكثافة التوزيع القطريللجسيم الواحد $D(r)$ ودالةالقيمة المتوقعة $\left\langle \frac{1}{r} \right\rangle$ لكل الحالات قيد الدراسة وتم برمجتها بواسطة برنامج الماثكاد .النتائج المستحصلة والمعطاه في الجداول والرسومات فسرت ونوقشت بشئ من التفصيل. تم التحقق من الثقة بهذا التقريب بمقارنة نتائجنا بالمتوفر من نتائج الأعمال السابقة.