ISSN: 0975-8585

Research Journal of Pharmaceutical, Biological and Chemical Sciences

Determination of the diamagnetic susceptibility $\chi_{diam.}$ and nuclear magnetic Shielding $\sigma_{magn.}$ constants for some atomic and ionic system.

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ABSTRACT

In this paper, two atomic parameter has been evaluated for several atomic and ionic systems: He, Li, Be, B, Ne, H^{-1} ,Li^{-1} , B^{+} , C^{+1},$N^{+3}$and C^{+4}.These parameters are, nuclear magnetic shielding $\sigma_{magn.}$ and diamagnetic susceptibility $\chi_{diam.}$ constants which are very important in the study of physical properties of the atoms and ions.For this purpose some expectation values of inter-electronic distances like $\langle r^{-1}\rangle$ and $\langle r^{2}\rangle$ which based upon the uncorrelated Hartree –Fock wave functions are used . All the results obtained in this work are shows the behaviors of $\sigma_{magn.}$ and $\chi_{diam.}$ are function of the atomic number Z within system .

Keywords: Hartree-Fock wave function ,magnetic shielding $\sigma_{magn.}$ and diamagnetic susceptibility $\chi_{diam.}$, atomic and ionic, Expectation values.

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INTRODUCTION

Recent developments in theoretical and computational methods ,have enabled the ab initio studies of a wide variety of molecular electric, magnetic, and optical properties. In particular, properties arising from the nonlinear response of the atomic and ionic systems to a combination of electric and magnetic fields can now be calculated[1].These properties are nuclear magnetic shielding constants $\chi'_{diam.}$ and $\sigma_{magn.}$ which are important in many applications ,like Nuclear Magnetic Resonance NMR imaging .The increasing interest is partly indebted to recent improvements and availability of computers and workstations[2].The diamagnetic susceptibility $\chi'_{diam.}$ of some elements and ions systems have been calculated in recent years by number of workers with employing several wave functions [3,4,5].A series of studies about the relativistic effects on the nuclear magnetic shielding constants [6–13].The aim of this paper is computing the diamagnetic susceptibility and Nuclear magnetic shielding constants for certain atomic ,positive and negative ions systems by depending on the some expectation values of inter-electronic distances $\langle r^{-1}\rangle$ and $\langle r^2\rangle$ from Richard and Larsson [14]as shown in table1. All the obtained results are analyzed and interpreted for these different systems .

Computational details

The Diamagnetic susceptibility $\chi'_{diam.}$

The magnetic susceptibility may be either positive or negative, when $\chi'_{magn.}$<0,the magnetization opposes the applied field and the magnetic induction in the medium is lower than it would be in a vacuum; such materials are classified as diamagnetic. But for $\chi'_{magn.}$>0, the magnetization adds to the applied field and increases the magnetic induction inside the material. Such substances are called paramagnetic. Therefore, we express it as the sum of a negative diamagnetic susceptibility, $\chi_{diam.}$, and a positive paramagnetic susceptibility, χ_{param}given by the equation[15] :

$$\chi_{magn.} = \chi_{diam.} + \chi_{param} = -\left(\frac{e^2\mu_0}{6m_e}\right)\langle r^2\rangle - \left(\frac{e^2\mu_0}{6m_e^2}\right)\sum_n \frac{|\ell_{0n}|^2}{\Delta E_{n0}} \text{..........(1)}$$

In which $\mu_0 = 4\pi \times 10^{-7} N/A^2$ is the permeability of vacuum space ,m$_e$ electron mass, ℓ_{0n} is the orbital angular momentum $\Delta E_{0n} = E_n^{(0)} - E_0^{(0)}$ represent the energy perturbation difference between the n and ground states .It should be emphasized that this paramagnetic contribution to the susceptibility has nothing to do with electron spin and unlike spin paramagnetic , is independent of temperature .The diamagnetic contribution is often called the Langevin term .Hence the susceptibility of a sample depends on the competition between the diamagnetic and paramagnetic contributions. In free atoms, the paramagnetic contribution is zero because we are free to choose the z-direction as the axis of quantization of the z-component magnetization;as a result ,the total molar susceptibility of a sample of atoms or ions is therefore[15]:

$$\chi_{diam.} = -\left(\frac{N_A e^2 \mu_0}{6m_e}\right)\langle r^2\rangle \text{...................(2)}$$

Equation 2 known as Langevin's formula provided that there are no unpaired spins. In the absence of spin all atom have a non-zero but small net diamagnetic susceptibility. As in eq.(1) , the susceptibility is the sum of diamagnetic and paramagnetic . In most molecules the former dominates, and most molecules without unpaired electron spins are diamagnetic, with molar susceptibilities proportional to $\langle r^2\rangle$. Only when there are low-lying excited electronic states may the orbital paramagnetic term dominate the Langevin's term and the molecule be weakly paramagnetic. In more compact form the equation 2 becomes[16,17]:

$$\chi_{diam.} = -\left(\frac{1}{6}\right)\alpha^2\langle\Psi \mid \sum_{i=1}^{n} r^2 \mid \Psi\rangle\ldots\ldots\ldots\ldots\ldots\ldots..(3)$$

Where $\alpha = 7.297353\times10^{-3}$ is the fine structure constant and the term $\langle r^2\rangle$ is the square of expectation values of electron distance relative to nucleus.

The Nuclear magnetic Shielding constant $\sigma_{magn.}$:

For the atomic and ionic system, the Nuclear Shielding constant[15,18] :

$$\sigma_{magn.} = \left(\frac{1}{3}\right)\alpha^2\langle\Psi \mid \sum_{i=1}^{n} r^{-1} \mid \Psi\rangle\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(4)$$

The equation (4) is called Lamb formula ,the magnetic of the diamagnetic contribution to the shielding is therefore depends inversely on the expectation distance of the electron $\langle r^{-1}\rangle$ from the nucleus [19].

RESULTS AND DISCUSSIONS

The diamagnetic susceptibility $\chi_{diam.}$ and nuclear magnetic shielding constants $\sigma_{magn.}$, we must determine $\langle r^2\rangle$ which requires the determination of the electron charge distribution within the system. However , the calculations involving quantum mechanics , that the concept of orbits replaced by wave function and quantities $\langle r^2\rangle$ and $\langle r^{-1}\rangle$ has a different significance, which based on the uncorrelated Hartree-Fock wave functions taken from [14],an given in the table (1).

Table (1):The expectation values of inter-electronic distances for several atomic and ionic systems (atomic units)[14].

Atom-ion	$\langle\frac{1}{r}\rangle$	$\langle r^2\rangle$
$_2$He	3.3746	2.3690
$_3$Li	5.716	18.633
$_4$Be	8.4089	17.3204
$_5$B	11.3795	15.8469
$_{10}$Ne	31.1133	9.3681
$_2$H^{-1}	1.3717	18.2799
$_4$Li^{-1}	5.870	87.79333
$_4$B^{+1}	10.9189	7.95050
$_5$C^{+1}	13.4229	4.6239
$_4$N^{+3}	15.9249	3.0412
$_2$C^{+4}	18.4216	2.1576

The diamagnetic susceptibility constants for several atomic and ionic systems are given in the table 2 are calculated by the equation 3.The present results may be summarized as follows:

The comparison of diamagnetic susceptibility $\chi_{diam.}$ for the electron systems such as that of He with $_2C^{+4}$ reveals that the their values with difference(8.9%) and $\chi_{diam.}$ of the He is greater due to the Columbic attraction force is less than that of $_2C^{+4}$.In other words, the latter experienced more force than the He, thus the result is the shrinking of the electron shells inward nucleus for $_2C^{+4}$. The same situation is correct for both $_4Li^{-1}$ and Li .

The comparison of diamagnetic susceptibility of positive and negative ions like :$_4Li^{-1}$and Li or $_2He$ and $_2H^{-1}$reveals that the $\chi_{diam.}$ values are proportional to the number of electrons within systems which increased predominately ,also from Langevin's equation its evident that the outer electrons(largest $\langle r^2 \rangle$) of electron systems, makes the largest contribution to the diamagnetic susceptibility .The results in table 2 ,shows that the nuclear magnetic shielding constants $\sigma_{magn.}$ decreases as Z decreases for both neutral atoms , positive and negative ions , this behavior can be explained due to the attraction force between the electrons and protons within nucleus.

Table(2):The expectation values of Diamagnetic susceptibility $\chi_{diam.}$ for several atomic and ionic systems (atomic units).

Atom-ion	$\chi_{diam.} \times 10^{-6}$	$\sigma_{magn.} \times 10^{-6}$
$_2He$	21.0247	5.2598
$_3Li$	165.3678	3.1053
$_4Be$	153.71855	2.11
$_5B$	140.64123	1.5598
$_{10}Ne$	83.14188	0.5705
$_2H^{-1}$	162.234	12.940
$_4Li^{-1}$	779.1568	3.0660
$_4B^{+1}$	70.650	1.62562
$_5C^{+1}$	41.03711	1.32236
$_4N^{+3}$	26.990	1.1146
$_2C^{+4}$	19.1487	0.9635

Concluding remarks

The results for $\chi_{diam.}$ and $\sigma_{magn.}$ refers to that the present method is valid for calculations of the diamagnetic shielding constants of light elements. The calculated results fairly well depends on the$\langle r^2 \rangle$and $\langle r^{-1} \rangle$ respectively , which in turns, depends atomic number Z within systems.

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