

Research article

# Spin-Orbit Coupling, Spin-Spin, NMR and Electric Properties of Hydrogen Chloride Molecule

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## Abstract

Research includes the study of the spin-orbit coupling, spin-spin, NMR, electronic structure and number electric properties such as ionization potential(IP), electron affinity(EA), electronegativity ( $\chi$ ), hardness( $\eta$ ), softness(S), electrophilic( $W$ ) and NMR spectroscopy of hydrogen chloride molecule by using Gaussian program 09 and Gauss view 5.08 program using density function (DFT) method B3LYP/6-311G (d,p).

Key words: spin-orbit coupling, spin-spin, NMR, electronic structure, electric properties, hydrogen chloride molecule, density function method .

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## Introduction

Hydrogen chloride is a diatomic molecule, consisting of a hydrogen atom H and a chlorine atom Cl connected by a covalent single bond [1]. Hydrogen chloride is a diatomic molecule, since the chlorine atom is much more electronegative than the hydrogen atom, the covalent bond between the two atoms is quite polar. This gas has the chemical formula HCl. At room temperature, it is colorless gas, which forms white fumes of hydrochloric acid upon contact with atmospheric humidity. Hydrogen chloride gas and hydrochloric acid are important in technology and industry [ 2]. Hydrochloric acid is a strong inorganic acid which used in many industrial processes. The application often determines the required product quality. Hydrochloric acid is used for

a large number of small-scale applications, such as, purification of common salt, and building construction. Oil production may be stimulated by injecting hydrochloric acid into the rock formation of an oil well, dissolving a portion of the rock, and creating a large-pore structure. Oil well acidizing is a common process in the North Sea oil production industry [3]. Many studies investigated calculation of spin-orbit coupling, spin-spin, NMR and electric properties. Used ab initio to study NMR spectroscopy for diatomic molecules [4]. Spin-orbit effects constitute a significant portion of relativistic effects for the studied molecules, and spin-spin between nuclei is of fundamental importance in magnetic resonance spectroscopy [5]. Spin-spin values were calculated of (HF, BF, KNa, and HCl) molecules[6]. A study of spin-orbit effect on the spectroscopic constant (bond length, dissociation energies and harmonic vibrational frequencies) for HX. X<sub>2</sub> (X=Cl, Br and I) and IZ (Z=F, Cl and Br) molecules[7]. The ionization potential, electron affinity, electronegativity, hardness, and electron excitation energy for diatomic molecules (Bc, Ne, Ar, HF) and organic molecules (NH<sub>3</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>=CH<sub>2</sub>) [8]. Finally, the calculation of spin-orbit coupling of the NaK 3<sup>3</sup> and 3<sup>1</sup> states, determination of the coupling constant and observation of quantum interference effects[9].

## Calculation

Calculation of spin-orbit coupling (SOC) values using of the following equation[10].

$$\text{SOC}(J) = L+S \quad \dots\dots\dots(1)$$

Where L represent the orbital angular momentum of molecule

Where S represent spin angular momentum of molecule

Ionization potential (IP) and electron affinity (EA) have been calculated by using equations [11].

$$\text{IP} = -E_{HOMO} \quad \dots\dots\dots(2)$$

$$\text{EA} = -E_{LUMO} \quad \dots\dots\dots(3)$$

Where E<sub>HOMO</sub> the energy of the highest occupied molecular orbital, while E<sub>LUMO</sub> the energy of the lowest unoccupied molecular orbital.

The electronegativity (χ) is defined as [12].

$$\chi = -(\text{IP}+\text{EA})/2 \quad \dots\dots\dots(4)$$

The hardness (η) has been calculated by using equation [12].

$$\eta = (\text{IP}-\text{EA})/2 \quad \dots\dots\dots(5)$$

Expresses the softness (S) and electrophilic (W) by the following equation [13].

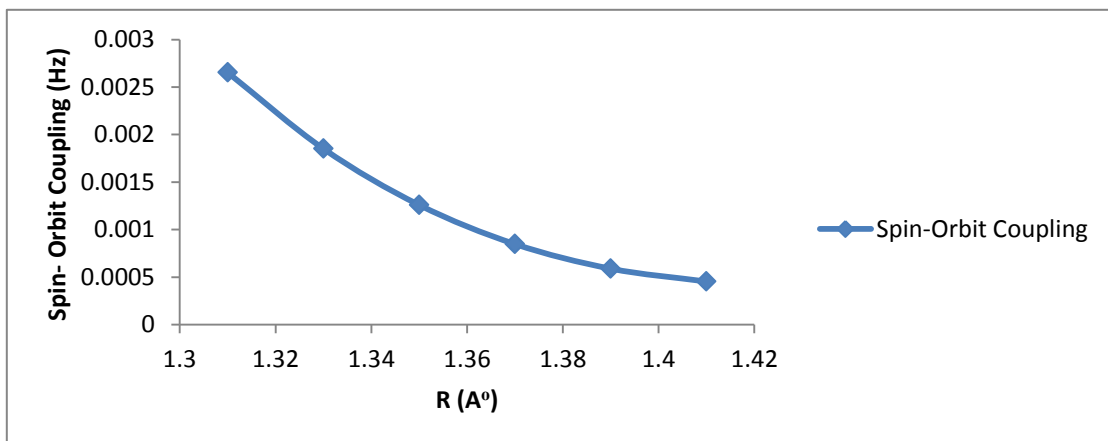
$$S = 1/2 \eta \quad \dots\dots\dots(6)$$

$$W = \chi^2 / 2 \eta \quad \dots\dots\dots(7)$$

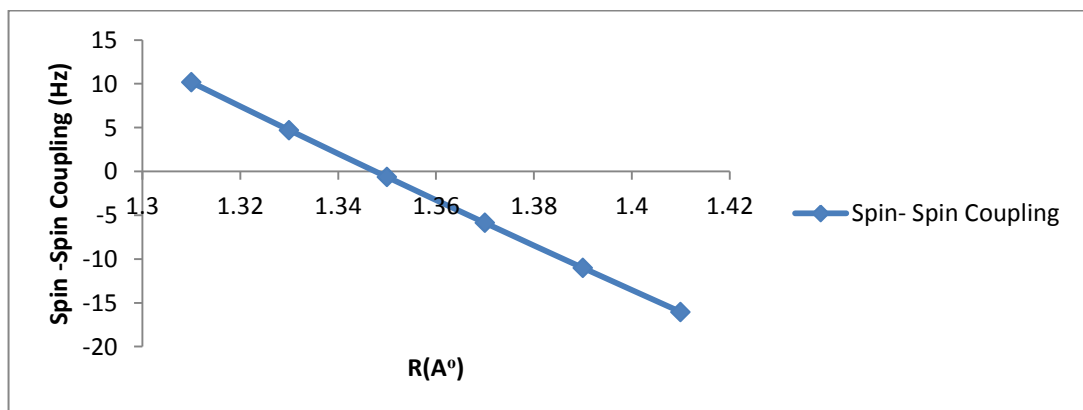
### Result and Conclusion

Table (1-1) : bond length (R) Measured in (Å), spin- orbit coupling, and spin- spin Measured in(Hz) for hydrogen chloride molecule.

R(Å)	Spin- orbit coupling (Hz)	Spin- spin (Hz)
1.31	0.00265293	10.168
1.33	0.00185115	4.70474
1.35	0.00125935	-0.643073
1.37	0.000848189	-5.87985
1.39	0.000589421	-11.0114
1.41	0.00045434	-16.0452



**Figure(1):** spin – orbit coupling of hydrogen chloride molecule



**Figure (2):** spin-spin of hydrogen chloride molecule

Table(1) and figure (1), shows the values of spin – orbit coupling for hydrogen chloride calculated by using Gaussian program 09 and Gauss view 5.08 program using density function (DFT) method, by using DFT, B3LYP/6-311G (d,p)[14] method, from this table and figure, it has been found that the values of spin –orbit coupling are decreasing with increasing the bond length between hydrogen and chloride atoms.

Figure (2) and table (1) shows the values of spin –spin coupling of hydrogen chloride calculated by using Gaussian program 09 and Gauss view 5.08 program using density function (DFT) method, by using DFT-B3LYP /6-311G (d,p)[14] method, from this figure and table (1) the values of spin- spin are decreasing with increasing the bond length, because the fluoride has high electronegativity, therefore chloride attached the electrons towered themselves this electrons lead to shielding the chloride for hydrogen atom, this refer that the spin-orbit coupling and spin-spin depending on the bond length.

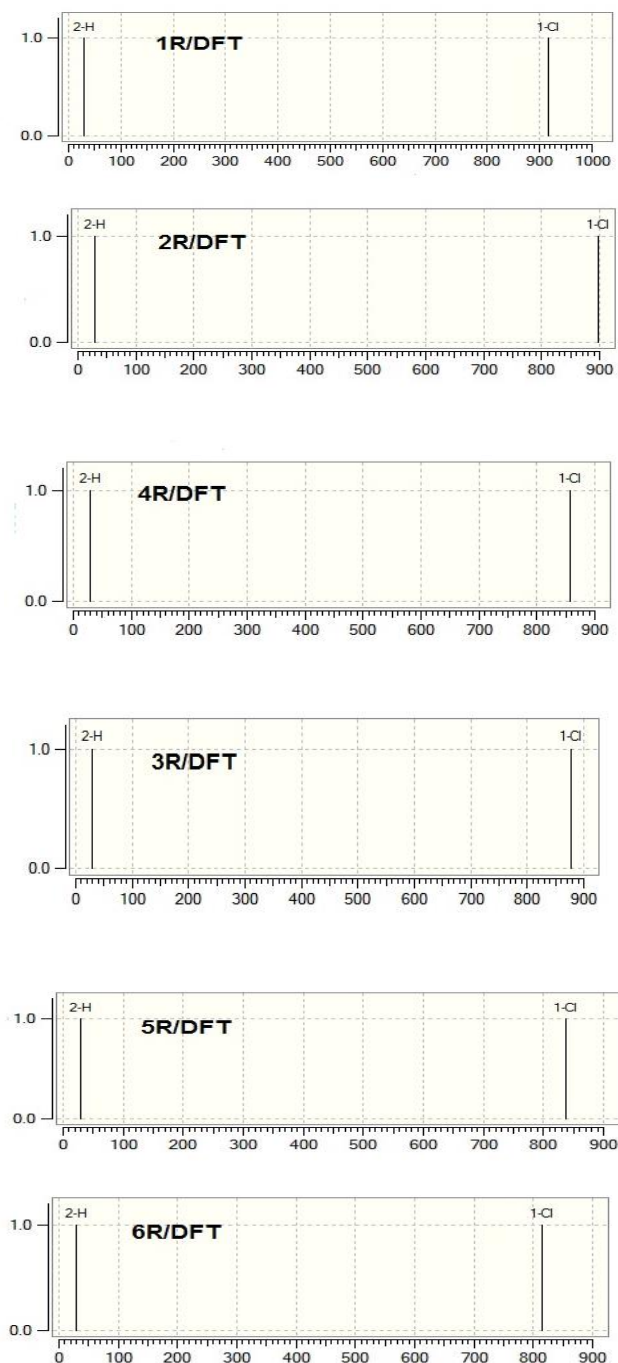
**Table (2):** boned length ( $A^\circ$ ),  $E_{HOMO}$  (eV),  $E_{LUMO}$ (eV), IP(eV),EA(eV),  $\chi$  (eV) , S(eV),  $\eta$  (eV) and W(eV) of hydrogen chloride molecule.

R( $A^\circ$ )	$E_{HOMO}$ (eV)	$E_{LUMO}$ (eV)	IP(Ev)	EA(eV)	$\chi$ (eV)	$\eta$ (eV)	S(eV)	W (eV)
1.31	-9.251196	-0.24163	9.251196	0.241634	4.746415	4.504781	0.110993	2.500505
1.33	-9.251196	-0.24163	9.251196	0.241634	4.746415	4.504781	0.110993	2.500505
1.35	-9.251196	-0.24163	9.251196	0.241634	4.746415	4.504781	0.110993	2.500505
1.37	-9.250924	-0.24191	9.250924	0.241906	4.746415	4.504509	0.111	2.500656
1.39	-9.250924	-0.24191	9.250924	0.241906	4.746415	4.504509	0.111	2.500656
1.41	-9.251196	-0.24191	9.251196	0.241906	4.746551	4.504645	0.110997	2.500724

Table (2) shows the values of ( $E_{HOMO}$ ,  $E_{LUMO}$ , IP, EA,  $\chi$   $\eta$  , S, and W) (eV) calculated by using DFT at basis set B3LYP/ 6-311G (d,p), it is clear from this table that the values of  $E_{HOMO}$  and  $E_{LUMO}$  are small difference with increasing of the bond length, also the values of all properties are slight increasing with increasing of bond length, except the values of hardness and softness are decreasing with increasing the bond length between hydrogen and chloride atoms.

Figure (3) shows the values of  $H^1$ NMR spectroscopy by using DFT method for hydrogen chloride molecule, from this figure found that the chemical shift proton of hydrogen is decreasing with increasing of the bond

length, also the chemical shift for the proton of chloride is decreasing for(1R-6R) hydrogen chloride molecule . The chemical shift at the range (915 -810) ppm and hydrogen at the range (30- 25) ppm, the chemical shift for chloride atom higher than that hydrogen atom because the chloride has high electronegativity therefore, the chloride attract the electrons towarded themselves, and diamagnetic shielding is important to study the NMR spectroscopy, where R is the bond length between hydrogen and chloride atoms.



Chemical shift (ppm)

**Figure (3):** Calculated of  $^1\text{H}$ NMR(1R-6R) of hydrogen chloride molecules by using B3LYP/6-311G(d,p) with increasing the bond length

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