

Comprehensive Analysis of Molecular Motion and Bonds of $C_{19}H_{21}ClN_2O$ Fungicide for Investigation of Unsteady Effects

Rajesh Kumar

Department of Physics, Indira Gandhi National Tribal University,
Amarkantak (MP), India

Abstract: This presented study is useful to enhance the ability of fungicides based on molecular theory. The crystallographic analysis of Pencycuron ($C_{19}H_{21}ClN_2O$) substance is done by us in the previous studies. Now, this work is extended as comprehensive analysis of molecular motion and bonding using Born Oppenheimer Approximation and molecular theory. So, this presented work is helpful to investigation of unsteady effects of the substance and possible solution for the desired result. Samples were prepared by a phase change process from liquid state to solid state at room temperature $30^\circ C$. The molecular structure of $C_{19}H_{21}ClN_2O$ substance was investigated by automatic computerized -4- Circles Enraf - Nonius CAD - 4- Diffractometer with help of SHELXL 97 and SHELXS program. The reduced mass and moment of inertia for diatomic molecules were evaluated by $\mu = \frac{m_1 \cdot m_2}{m_1 + m_2}$ and μr^2 respectively for bond analysis.

Keywords: Unsteady effects, Molecular motion, Born Oppenheimer Approximation, Inter-atomic distance, Diffractometer

1. INTRODUCTION

The $C_{19}H_{21}ClN_2O$ fungicide is a compound of molecules which is used in botanical and agriculture purpose for control of fungal [1]. Molecular structure and packing diagram of $C_{19}H_{21}ClN_2O$ fungicide were reported by J. Chauhan et al. [2]. In the late 1800s and early 1900s were developed new theories of atomic and molecular for interpretation of atom and molecular [3]. The wave function and quantum number associated with moving molecules for confirming motion as electronic, vibration and rotational motion. On the basis of motion of molecules there are three kinds of energy named as electronic energy E_e , vibrational energy E_v and rotational energy E_r . There are various energy levels and transition levels are possible due to involvement of quantum numbers with motion. Quantum numbers $v, j = 0, 1, 2, 3, 4$ are associated with vibration and rotational motion respectively. In quantum theory, the wave function is also attached with each motion. The electron transition is occurred between two energy states; it will absorb or emit the energy as a form of electromagnetic radiation [4]. The Born Oppenheimer Approximation (BOA) is separated motion of molecules as electronic and nuclear motion [5]. Therefore, vibrational and rotational motion considered under nuclear motion. The $C_{19}H_{21}ClN_2O$ substance has bond length, bond angles and torsion angles which are affecting its impact due to apropos motions and transitions.

1.1 Research Methodology

The chemical structure of $C_{19}H_{21}ClN_2O$ substance is providing the information of molecular position, which is helpful for analysis. Solid sample were prepared from liquid by natural evaporation process. The crystallographic structure was investigated by CAD 4 circle - diffractometer at SAIF, IIT, Madras at 293 K. The molecular structure provides the information of molecules position, bonds and length. Based on the bond and bond length, we evaluated the reduced mass and moment of inertia by formula. The molecular has vibrational and rotational motion. Therefore, inter-atomic distance (r), moment of inertia (μ) and attraction force has been changed due to vibrational motion of atoms. This change is affected by the impact of $C_{19}H_{21}ClN_2O$ substance. Another thing is that the electron transitions from energy level to various excited states, so electrons will be delocalized and simultaneously bond length has been changed. Impact of bond length may be responsible for the unsteady effect of the substance. Based on the value of moment of inertia and reduced mass, we can find the variation of the compounds due to molecular motion. The absorption and transition rate of $C_{19}H_{21}ClN_2O$ substance will be affected by electron transition and energy levels. During motion, the possible energy or total energy of the molecules expressed as [6].

$$E_{\text{Total}} = E_{\text{spin}} + E_{\text{nucleus}} + E_{\text{transition}} + E_{\text{electronic}} + E_{\text{rotational}} + E_{\text{vibrational}}$$

The temperature variation and doping can change the total energy of molecules. Based on the quantum model, the wave function is associated with each motion, and they explain motion, energy and amplitude as well. This hypothesis is useful for investigation of the unsteady effect of concerned substances.

1.2 Theoretical Hypothesis

The basic information like reactivity, structure energy and stability is provided by vibrational motions of molecules or chemical reactions [7]. Molecular motion was proved by Nuclear Magnetic and Resonance (NMR) in 1997 by G Palmer [8]. The molecule has spin, transition, nucleus, electronic, rotational and vibrational motions, which all of them release energy. When two atoms interact with each other and connect with distance r . Due to vibrational motion this bond length will be changed, so accordingly attractiveness is also changed. Reduced mass

of the diatomic system depends on mass of concerned atoms. When atoms or molecules are rotating with their own axis, this motion has a moment of inertia.

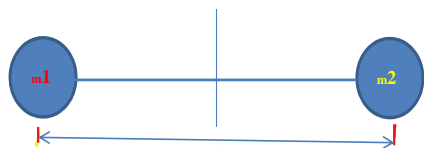


FIGURE 1: Schematic representation of bond length (r) of diatomic molecules.

Reduced mass of diatomic molecules is

$$\mu = \frac{m_1 \cdot m_2}{m_1 + m_2} \quad [1]$$

Where, m_1 and m_2 is masses of atoms

The moment of inertia evaluated by

$$I = \mu r^2 \quad [2]$$

Here, μ is the reduced mass and r is the distance between two atoms.

The rotational energy (E_r) of diatomic molecules is inversely proportional to the moment of inertia, and it is varying with rotational quantum number J ($= 1, 2, 3, \dots$) and rotational constant B . We have various energies level with j and B , hence possible electron transitions will be occurred in these energies.

$$E_r = \frac{1}{\mu r^2} = \frac{1}{I} \quad [3]$$

The chemical structure of $C_{19}H_{21}ClN_2O$ substance is shown in figure 2, and it provides ideas of molecular position, compounds and bonds etc. During three-

dimensional motion or transition, related bond length, bond angle, reduced mass and moment of inertia will vary or change. In the Pencycuron, we have two benzene rings with six molecules for each.

Chemical weight of $C_{19}H_{21}ClN_2O = 328.6547$ g/mol.

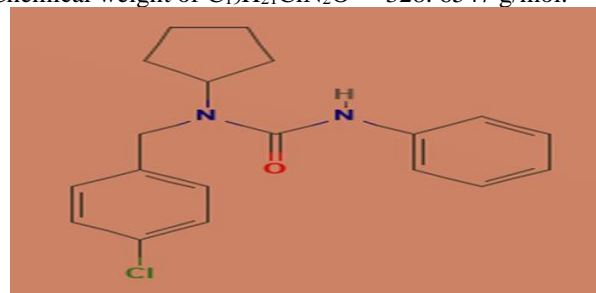


FIGURE 2: Chemical structure of $C_{19}H_{21}ClN_2O$ substance in 2D (PubChem).

The complex molecules are present in $C_{19}H_{21}ClN_2O$ substance which will affect its results. Further, the impact of substances depends on electronic transition, absorption and transmission rates. The optical excitations are providing information of the electronic states of the complex molecules based on the study of emission [9]. Therefore, bond length may decrease or increase based on type of motions. Experimental bond lengths basically depend on molecular vibration and computational bond lengths are available. These both bond lengths have differences in range $1000 - 100 \text{ \AA}$ due to temperature variation [10].

TABLE 1: Description of associated atoms with $C_{19}H_{21}ClN_2O$ substance

Atom's Name	Atomic mass (in u)	No. of Atoms	Coding of atom*
Carbon	12.011	C 19	C ₁ , C ₂ , C ₃ , C ₄ , C ₅ , C ₆ , C ₇ , C ₈ , C ₉ , C ₁₀ , C ₁₁ , C ₁₂ , C ₁₃ , C ₁₄ , C ₁₅ , C ₁₆ , C ₁₇ , C ₁₈ and C ₁₉
Nitrogen	14.007	N 2	N ₁ , N ₂
Chlorine	35.435	Cl 1	Cl ₁
Oxygen	15.999	O- 1	O ₁

*Atom's coding is required for analysis of substance.

3. RESULTS AND DISCUSSION

In the molecular structure, we have two benzene rings present in $C_{19}H_{21}ClN_2O$ substance, each ring having 6 molecules and connected in ring form. The associated molecules with ring is (Ring 1) C₂, C₃, C₄, C₅, C₆, C₇ (Ring 1) and C₁₄, C₁₅, C₁₆, C₁₇, C₁₈ and C₁₉ (Ring 2). When these rings are in motion, the bond length has been changed along with the moment of inertia. We are showing bonds, bond length, reduced mass and moment of inertia in table 2. The lowest bond length is $1.231 \times 10^{-10} \text{ m}$ for C₇- O₁ and highest is $1.745 \times 10^{-10} \text{ m}$ for C₁₇- Cl₂. We observed that various bond lengths for the same bond due to vibrational and electronic motion of molecules such as $1.386 \times 10^{-10} \text{ m}$, $1.515 \times 10^{-10} \text{ m}$ and $1.723 \times 10^{-10} \text{ m}$ is for C₁ - C₂, C₉ - C₁₀ and C₆- C₁ respectively. Reduced mass of C- C bond is $9.968 \times 10^{-27} \text{ Kg}$ that is lowest in the whole compound and C₁₇ - Cl₂ is $14.895 \times 10^{-27} \text{ Kg}$ (highest). The value of μ is different for the various compounds, and it is related to the

moment of inertia of the concerned diatomic molecules. Hence, moment of inertia $I = \mu r^2$ it also varies with μ . By evaluation, we obtained a moment of inertia for C₇ - O₁ is $17.261 \times 10^{-47} \text{ kg-m}^2$ and C₁₇- Cl₂ is $45.355 \times 10^{-47} \text{ kg-m}^2$. The moment of inertia depends on reduced mass and inter-atomic distance [11]. The variation of moment of inertia with bond length due to variable temperature we showed on figure 4. This variation indicates that all compounds and bonds are not active properly; it means some bonds are inactive in nature. Similar, moment of inertia vs reduced mass is represented on figure 5 for variation of compounds.

When reduced mass is increased or decreased, accordingly these impacts reflect on I . As collected data the bond length not equal is with the same bond due to nuclear and electronic motions. The Born Oppenheimer Approximation says that both motions can be separate and electronic and nuclear motion has wave function ψ_e and ψ_n

respectively [12]. During molecules motion, the absorption and transition rate we can find by the rotational, vibrational and electronic motions of molecules for study of excitation and energy levels. The result of $C_{19}H_{21}ClN_2O$ substance depends on all above parameters like I , μ , r , E (E_r , E_v , E_e), T and variation of all of them. For enhancement of output, we can add doping with suitable material or remove unwanted and inactive compounds but this is not limited.

Also, we can use another way for the solution of the problem by chemical, optical, electrical and physical properties based on the fungicide analysis in Nano-particles form. This presented paper is helpful to improve of $C_{19}H_{21}ClN_2O$ substance based on the physical aspect only for getting desired outcome for good result of fungicides in the crops.

TABLE 2: Data collection and evaluation

Bond's name		Atomic mass of atom 1 (In u)	Atomic mass of atom 2 (In u)	Bond length (r) (In 10^{-10} m)	Reduce mass (In 10^{-27} Kg)	$I = \mu r^2$ (In 10^{-47} kg-m ²)
Atom names (1)	Atom names (2)					
C ₁	N ₁	12.011	14.007	1.412	10.737	21.406
C ₁₄	C ₁₅	12.011	12.011	1.381	9.968	19.010
C ₁₃	N ₂	12.011	14.007	1.452	10.737	22.636
C ₁₅	C ₁₆	12.011	12.011	1.383	9.968	19.065
C ₇	O ₁	12.011	15.999	1.231	11.391	17.261
C ₁₆	C ₁₇	12.011	12.011	1.363	9.968	18.518
C ₇	N ₂	12.011	14.007	1.360	10.737	19.859
C ₁₇	C ₁₈	12.011	12.011	1.364	9.968	18.545
C ₇	N ₁	12.011	14.007	1.370	10.737	20.152
C ₁₇	Cl ₂	12.011	35.435	1.745	14.895	45.355
C ₈	N ₂	12.011	14.007	1.478	10.737	23.454
C ₁₈	C ₁₉	12.011	12.011	1.383	9.968	19.065
C ₁	C ₂	12.011	12.011	1.386	9.968	19.148
C ₂	C ₃	12.011	12.011	1.376	9.968	18.873
C ₃	C ₄	12.011	12.011	1.363	9.968	18.518
C ₄	C ₅	12.011	12.011	1.377	9.968	18.900
C ₅	C ₆	12.011	12.011	1.383	9.968	19.065
C ₆	C ₁	12.011	12.011	1.723	9.968	29.592
C ₈	C ₉	12.011	12.011	1.516	9.968	22.909
C ₈	C ₁₂	12.011	12.011	1.533	9.968	23.425
C ₉	C ₁₀	12.011	12.011	1.515	9.968	22.878
C ₁₀	C ₁₁	12.011	12.011	1.495	9.968	22.278
C ₁₁	C ₁₂	12.011	12.011	1.504	9.968	22.547
C ₁₃	C ₁₄	12.011	12.011	1.518	9.968	22.969
C ₁₄	C ₁₉	12.011	12.011	1.380	9.968	18.983

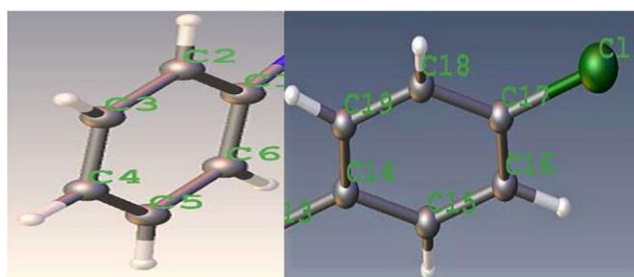


FIGURE 3: Benzene rings of Pencycuron substance, J. Chauhan et al, (2013), IJSER, 4(11), 988-998.

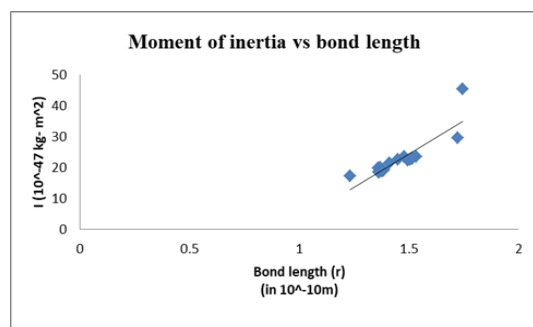


FIGURE 4: Variation of moment of inertia with bond length.

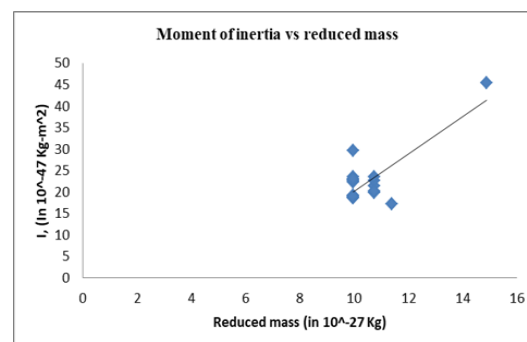


FIGURE 5: Moment of inertia vs reduced mass

Table 3: Lowest and highest value of molecules bond

S. No.	Parameter's name	Lowest value and concerned bond's name	Highest value and concerned bond's name
1	Bond length	1.231×10^{-10} m C ₇ -O ₁	1.745×10^{-10} m C ₁₇ -Cl ₂
2	Reduced mass	9.968×10^{-27} Kg C - C	14.895×10^{-27} Kg C ₁₇ -Cl ₂
3	Moment of inertia	17.261×10^{-47} kg-m ² C ₇ -O ₁	45.355×10^{-47} kg-m ² C ₁₇ -Cl ₂

4. CONCLUSION

We find the unsteady effects of C₁₉H₂₁ClN₂O substance based on the molecule's theory. The motion of molecules may change the bond length, moment of inertia and transition rate of the fungicides. Sometimes, elements and compounds is inactive mode due to impact of climate and electron delocalization. This study is very useful to find the unwanted compounds. So we can resolve this problem by substitution of suitable elements and doping. Hence, we can enhance the ability of fungicides by this reported work and may achieve desired outcome in the crops and flowers. The transmission and absorption rates of fungicides can be increase by molecular motion. So, fungicides will be more effective to control of fungal than we can obtain good result.

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