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RESEARCH ARTICLE OPEN ACCESS

Comprehensive Analysis of Molecular Motionand Bonds of $C_{19}H_{21}CLN_2O$ Fungicide forInvestigation of Unsteady Effects

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ABSTRACT: This presented study is useful to enhance the abilityof fungicides based on molecular theory. The crystallographicanalysis of Pencycuron ($C_{19}H_{21}ClN_2O$) substance is done by usinthepreviousstudies.Now,thisworkisextendedascomprehensiveanalysisofmolecularmotionandbondingusingBornOppenheimerApproximationandmoleculartheory. So, this presented work is helpful to investigation ofunsteady effects of the substance and possible solution for thedesiredresult.Sampleswerepreparedbyaphasechangeprocess from liquid state to solid state at room temperature 30^0C. The molecular structure of $C_{19}H_{21}ClN_2O$ substance wasinvestigated by automatic computerized -4- Circles Enraf -Nonius CAD – 4- Diffractometer with help of SHELXL 97 andSHELXSprogram.Thereducedmassandmomentofinertia fordiatomicmoleculeswereevaluatedby $\mu = \frac{m1 * m2}{m1+m2}$ and μr^2 respectively forbondanalysis.

Keywords:Unsteadyeffects,Molecularmotion,BornOppenheimerApproximation,Inter-atomicdistance,Diffractometer

I. INTRODUCTION

The$C_{19}H_{21}ClN_2O$fungicideisacompound ofmolecules which is use in botanical and agriculture purposefor control of fungal [1]. Molecular structure and packingdiagramof$C_{19}H_{21}ClN_2O$fungicidewererep ortedbyJ.Chauhan et al. [2]. In the late 1800s and early 1900s weredevelopednewtheoriesofatomicandmolecularfo rinterpretationofatomandmolecular[3].Thewavefun ctionandquantumnumberassociatedwithmovingmol ecules for confirming motion as electronic, vibrationand rotational motion. On the basis of motion of moleculesthere are three kinds of energy named as electronic energyE_e, vibrational energy E_V and rotational energy E_r. There arevarious energy levels and transition levels are possible dueto involvement of quantum numbers with motion. Quantumnumbers v, j = 0, 1,2,3,4 are associated with vibration androtationalmotionrespectively.Inquantumtheory,t hewavefunctionisalsoattachedwitheachmotion.Thee lectron transition is occurred between two energy states; itwill absorb or emit the energy as a form of electromagneticradiation[4].TheBornOppenheimer Approximation(BOA) is separated motion of molecules as electronic andnuclear motion [5]. Therefore. Vibrational and rotationalmotion considered under nuclear motion. The $C_{19}H_{21}ClN_2O$substance has bond length, bond angles and torsion angleswhich are affecting its impact due to apropos motions andtransitions.

1.1 ResearchMethodology

The chemical structure of $C_{19}H_{21}ClN_2O$ substanceis providing the information of molecular position, which ishelpfulforanalysis.Solidsamplewerepreparedfroml iquid by natural evaporation process. The crystallographicstructure was investigated by CAD 4 circle - diffractometerat SAIF, IIT, Madras at 293 K. The molecular structure areprovides the information of molecules position, bonds andlength. Based on the bond and bond length, we evaluatedthe reduced mass and moment of inertia by formula. Themolecular has vibrational and rotational motion. Therefore,inter-atomicdistance(r),momentofinertia(μ)andattraction force has been changed due to vibrational motionofatoms.Thischangeisaffectedbytheimpactof $C_{19}H_{21}ClN_2O$ substance. Another thing is that the electrontransitions from energy level to various excited states, soelectronswillbedelocalizedandsimultaneouslybon dlength has been changed. Impact of bond length may beresponsible for the unsteady effect of the

substance.
Basedonthevalueofmomentofinertiaandreducedmass,wecan find the variation of the compounds due to molecularmotion. The absorption and transition rate of $C_{19}H_{21}ClN_2O$substance will be affected by electron transition and energylevels.During motion, the possibleenergy or totalenergyofthe moleculesexpressedas[6].

$E_{Total}=E_{spin}+E_{nuclues}+E_{transition}+E_{electronic}+E_{rotational}+E_{vibrational}$

The temperature variation and doping can changethetotalenergyofmolecules.Basedonthequantummodel, the wave function is associated with each
motion,andtheyexplainmotion,energyandamplitude as well.This hypothesis is useful for investigation of the unsteadyeffectof concernedsubstances.

1.2 TheoreticalHypothesis

Thebasicinformationlikereactivity,structureenergy and stability is provided by vibrational motions ofmolecules or chemical reactions [7]. Molecular motion wasprovedbyNuclearMagneticandResonance(NMR)in1997 by G Palmer [8]. The molecule has spin, transition,nucleus,electronic,rotationalandvibrationalmotions,which all of them release energy. When two atoms interactwitheachotherandconnectwithdistancer.Due tovibrational motion this bond length will be changed,
soaccordinglyattractivenessisalsochanged.Reduced mass

ofthediatomicsystemdependsonmassofconcernedatoms. When atoms or molecules are rotating with theirown axis, thismotionhasa momentofinertia.

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

Reducedmassofdiatomicmoleculesis

dimensional motion or transition, related bond length, bondangle, reduced mass and moment of inertia will vary orchange. In the Pencycuron, we have two benzene rings withsix moleculesfor each. ChemicalweightofC19H21ClN2O=328.6547 g/mol.

$$\mu=\frac{m1*m2}{m1+m2}$$

Where,$m_1$and$m_2$ismassesofatomsThemomentofine

rtiaevaluated by
[1]

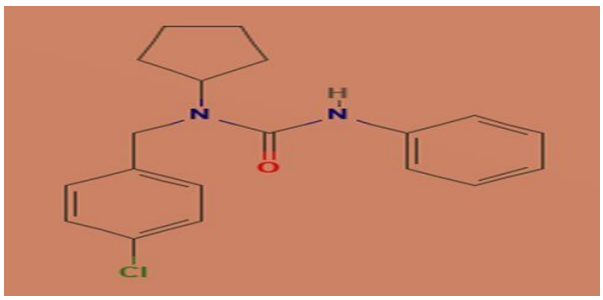

FIGURE 2: Chemical structure of $C_{19}H_{21}ClN_2O$ substance in 2D(PubChem).

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

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

The rotational energy(Er) of diatomic moleculesis inversely proportional to the moment of inertia, and it isvaryingwithrotationalquantumnumberJ(=1,2,3) and rotational constant B. We have various energies levelwith j and B, hence possible electron transitions will beoccurred inthese energies.

The complex molecules are present in $C_{19}H_{21}ClN_2O$substancewhichwillaffectitsresults. Further,theimpactofsubstancesdependsonelectronict ransition, absorption and transmission rates. The opticalexcitationsareprovidinginformationoftheelec tronicstatesofthecomplexmoleculesbasedonthestudy ofemission[9].Therefore,bondlengthmaydecreaseori ncreasebasedontypeofmotions.Experimentalbondle ngthsbasically dependon molecularvibration and

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

computationalbondlengthsareavailable.Thesebothb ond lengthshavedifferencesinrange1000-100Ådueto

The chemical structure of $C_{19}H_{21}ClN_2O$ substanceis shown in figure 2, and it provides ideas of molecularposition,compoundsandbondsetc.Duringt hree-temperaturevariation[10].

TABLE1:Descriptionofassociatedatomswith$C_{19}H_{21}ClN_2O$substance

Atom'sName	**Atomic mass(in u)**	**No.of Atoms**	**Codingofatom***
Carbon	12.011	C 19	C1,C2,C3,C4C5,C6,C7,C8,C9C10, C11,C12,C13,C14C14,C15,C16,C17,C18 andC19
Nitrogen	14.007	N2	N1,N2
Chlorine	35.435	Cl1	Cl1
Oxygen	15.999	O- 1	O1

*Atom'scodingisrequiredforanalysisofsubstance

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II. RESULTS AND DISCCUISSION

In the molecular structure, we have two benzenerings present in $C_{19}H_{21}ClN_2O$ substance, each ring having 6moleculesandconnectedinringform.Theassociated molecules with ring is (Ring 1) C2, C3, C4, C5, C6, C7 (Ring1) and C14, C15, C16, C17, C18 and C19 (Ring 2). When theseringsareinmotion,thebondlengthhasbeenchang edalong with the moment of inertia. We are showing bonds,bondlength,reducedmassandmomentofinertia intable

1. The lowest bond length is $1.231 * 10^{-10}$ m for C7- O1 andhighest is $1.745 * 10^{-10}$ m for C17-Cl2. We observed thatvarious bond lengths for the same bond due to vibrationaland electronic motion of molecules such as $1,386 * 10^{-10}$ m,$1.515 * 10^{-10}$ m and $1.723 * 10^{-10}$ m is for C1 – C2, C9 – C10and C6- C1respectively. Reduced mass of C- C bond is$9.968 * 10^{-27}$ Kg that is lowest in the whole compound andC17– Cl2is $14.895* 10^{-27}$ Kg (highest). The value of μ isdifferentforthevariouscompounds,anditisrelatedtot he moment of inertia of the concerned diatomic molecules.Hence, moment of inertia $I = \mu r^2$ it also varies with μ. Byevaluation, we obtained a moment of inertia for C7 – O1 is$17.261*10^{-47}$kg-m^{2}andC17-Cl2is$45.355*10^{-47}$kg-m^2.

Themomentofinertiadependsonreducedmassandinte r-atomic distance [11]. The variation of moment of inertiawithbondlength dueto variabletemperature weshowedon figure 4. This variation indicates that all compounds andbonds are not active properly; it means some bonds areinactive in nature. Similar, moment of inertia vs reducedmassisrepresented onfigure5forvariationofcompounds.

Whenreducedmassisincreasedordecreased,accordin gly these impacts reflect on I. As collected data thebond length not equal is with the same bond due to nuclearandelectronicmotions.TheBornOppenheime rApproximation says that both motions can be separate andelectronicandnuclearmotionhaswavefunctionψ**e** andψn respectively [12]. During molecules motion, the absorptionand transition rate we can find by the

rotational, vibrationaland electronic motions of molecules for study of excitationand energy levels. The result of $C_{19}H_{21}ClN_2O$ substancedepends 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,wecanadddopingwithsuitablematerialorremoveunwantedandinactivecompoundsbutthisisnotlimited.

Also,wecanuseanotherwayforthesolutionoftheproblembychemical,optical,electricalandphysicalpropertiesbasedonthefungicideanalysisinNano-particlesform.Thispresentedpaperishelpfultoimproveof$C_{19}H_{21}ClN_2O$substancebasedonthephysicalaspectonlyforgettingdesiredoutcomeforgoodresultoffungicidesinthe crops.

TABLE2:Datacollection andevaluation

Bond'sname		Atomicmass ofatom1 (Inu)	Atomic mass ofatom2 (Inu)	Bond length (r)(In1 0^{-10}m)	Reducemass(In 10^{-27}Kg)	$I=\mu r^2$ ($In10^{-47}$kg-m^2)
Atom names(1)	Atomnames(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

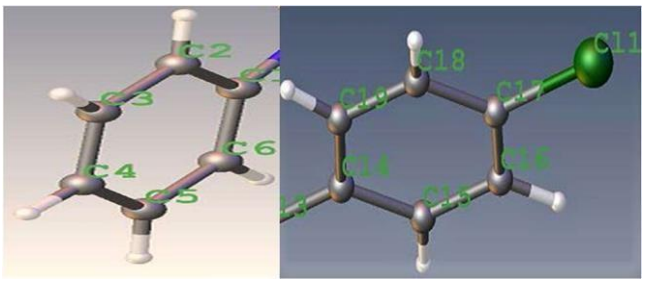

FIGURE3:BenzeneringsofPencycuronsubstance,J.Chauhanetal,(2013),IJSER,4(11),988-998.

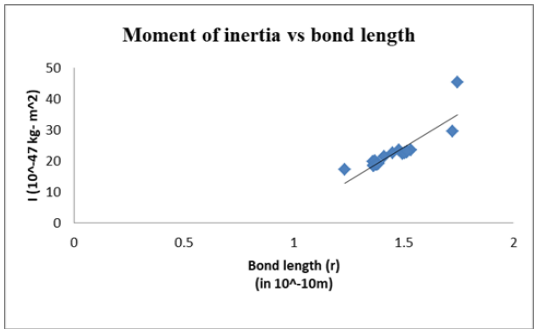

FIGURE4:Variationofmomentofinertiawithbondlength.

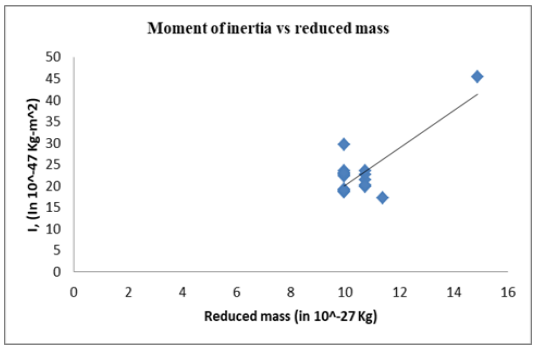

FIGURE5:Momentofinertiavsreducedmass

Table3:Lowestandhighestvalue ofmoleculesbond

S. No.	**Parameter'sname**	**Lowestvalueandconcernedbond'sname**	**Highestvalueandconcernedbond'sname**
1	Bondlength	$1.231*10^{-10}$m C7- O1	$1.745*10^{-10}$m C17-Cl2
2	Reducedmass	9.968 * 10-^{27} KgC-C	14.895*10-^{27}Kg C17-Cl2
3	Momentofinertia	$17.261*10^{-47}$kg-m^2 C7–O1	$45.355*10^{-47}$kg-m^2 C17-Cl2

III. CONCLUSION

WefindtheunsteadyeffectsofC19H21ClN2 Osubstance based on the molecule's theory. The motion ofmolecules may change the bond length, moment of inertiaand transition rate of the fungicides. Sometimes, elementsand compounds is inactive mode due to impact of climateandelectrondelocalization.Thisstudyisveryus efultofindtheunwantedcompounds.Sowecanresolvet hisproblem by substitution of suitable elements and doping.Hence, we can enhance the ability of fungicides by thisreportedworkandmayachievedesiredoutcomeint hecrops and flowers. The transmission and absorption rates offungicidescanbeincreasebymolecularmotion.So,f ungicides will be more effective to control of fungal thanwecanobtaingoodresult.

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