

DFT and Spectral Analysis of 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione

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ABSTRACT

In this work vibrational Spectral analysis of 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione (5H3HM1D) have been investigated by theoretical vibration data indicated the presence of variable functional groups with the total of molecule the equilibrium geometry, bonding features, harmonic vibration frequency. FT-IR and Raman intensities have been calculated with the help of density functional theory methods. The assignments of vibration spectra have been carried out the normal co-ordinate's analysis following the scaled quantum mechanical force field calculations. The First hyperpolarizability(β_{tot}) of the novel molecules system and related properties (μ , α and $\Delta\alpha$) are calculated using B-3LYP/6-31+G (d) and B3LYP/6-311++G(d, p) method on the finite-field approach. The calculated HOMO and LUMO energies show that charger transfer occurs within the molecule. Information about the size, shape, charge density distribution and site of chemical reactivity of the molecules has been obtained by mapping electrons density surface with molecular electrostatics potential.

Keywords: Vibrational Spectra, DFT Calculations, HOMO-LUMO, MEP Surface.

I. INTRODUCTION

Indole is a fragrant heterocyclic compound comprising of intertwined benzene and pyrrole rings through the 2-and 3-places of the pyrrole part. Since its first combination in 1866, indole was found in numerous characteristic items like parasitic metabolites and marine normal items in different bioactive agrochemicals and drugs [1]. The nitrogen particle present in fragrant heterocycles can communicate with the other sub-atomic focuses through hydrogen security [2]. Indole subsidiaries have unmistakable property of addressing the construction of peptides and restricting reversibly to catalyst [3]. Because of this property, indole subordinates clear an astounding method to find novel medications on natural focuses with an alternate method of activity. Indole containing compounds are notable to show an assortment of pharmacological exercises, for example, mitigating [4], cancer prevention agent [5] antidiabetic [6], antiviral [7], antifungal [8], antibacterial [9], and anticancer [10]. Indole may be utilized as a promising platform in the advancement of novel nicotinic opponents [11]. Characteristic cell reinforcements can dodge or if nothing else fundamentally diminish the peroxidation of lipids by free extremists, which are identified with an assortment of issues and infections [12]. Indole is a chromophore of the amino corrosive tryptophan that has acquired obvious premium of numerous scientists to research the instruments of the different photophysical responses going on inside tryptophan particle in different conditions. Because of these properties bright emanation range and fluorescence lifetime to its nearby environmental factors, makes it a fundamental boundary in understanding protein usefulness just as dissolvable availability [13]. In the new time, endeavours have been fixated on the fluorescent conduct of indole compounds in non-fluid conditions. It has been discovered that expansion of modest quantity of alcohols to a non-polar

dissolvable would result to striking changes in the emanation spectra of indole compounds. This wonder has been ascribed to the development of exciplexes between particle of indole and that of polar added substance [14]

II. MATERIALS AND METHODS

The sample 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione (5H3HM1D) in the white crystal form was provided by the Fluorochem Ltd, (UK) with a purity of greater than 98% and it was used as such without further purification. The FT-Raman spectrum of 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione was recorded using 1064 nm line of Nd:YAG laser as excitation wavelength in the region 3500-100 cm^{-1} on a Thermo Electron Corporation model Nexus 670 spectrometer equipped with FT-Raman module accessory. The FT-IR spectrum of 5H3HM1D was recorded in the frequency region 4000-400 cm^{-1} on a Nexus 670 spectrometer equipped with an MCT detector, a KBr pellet technique.

III. COMPUTATIONAL DETAILS

In order to model the structure and to compare the performance of DFT methods on 5H3HM1D, geometry optimization followed by vibrational frequency calculations were performed at the DFT/B3LYP/6-31+G(d) and B3LYP/6-311++G (d,p) using the GAUSSIAN 09W [15] without any constraint on the geometry. Transformation of force field from Cartesian to symmetry coordinate, scaling, subsequent normal coordinate analysis and calculations of PED, IR and Raman intensities were made on a PC with the version V7.0 of the MOLVIB program written by Sundius [16,17]. By combining the results of the GAUSSVIEW [18] with symmetry considerations, along with the available related molecules, vibrational frequency assignments were made with a high degree of accuracy.

Predictions of Raman intensities

The Raman activities(SR) calculated with the Gaussian 09W program were converted to relative Raman intensities (IR) using the following relationship derived from the basic theory of Raman scattering [19-21].

$$I_R = \frac{f(v_0 - v_i)4 S_R}{v_i \left[1 - \exp\left(-\frac{hcv_i}{kT}\right) \right]}$$

where v_0 is the laser exciting frequency in cm^{-1} (in this work, we have used the excitation wave number $v_0=9398.5 \text{ cm}^{-1}$, which corresponds to the wavelength of 1064nm of Nd:YAG laser), v_i is the vibrational wavenumber of the i^{th} normal mode (in cm^{-1}) and S_R is the Raman scattering activity of the normal mode v_i , (is the constant equal to 10^{-12}) is a suitably chosen common normalization factor for all peak intensities $h, k, c,$ and T are Planck constant, Boltzmann constant, speed of light, and temperature in Kelvin, respectively.

IV. RESULT AND DISCUSSION

Molecular Geometry

The streamlined calculations of the compound 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione in Fig. 1 are performed by DFT/B3LYP level with 6-31G+(d) and 6-311G++(d,p) premise set. The advanced primary boundaries bond lengths, bond points and dihedral points of title compound. The upgraded bond boundaries of 5H3HM1D determined by DFT/B3LYP techniques utilizing 6-31G+(d) and 6-311G++(d,p) premise set are contrasted and the comparable sort of atom [22] structure has been addressed. From the hypothetical qualities we can track down that a large portion of the upgraded bond lengths and bond points. The determined bond distances of C_1C_2 , C_2C_3 , C_3C_4 , C_4C_5 and C_5C_6 shows the distinction as 0.1 Å.

Vibrational Analysis

In the current investigation, the spectroscopic mark of 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione has been examined by the hypothetical FT-IR and FT-Raman spectra. The title compound comprises of 29 atoms, accordingly it has 81 vibrational levels of opportunity under C1 point group. In the current investigation, every one of the 81 ordinary methods of vibrations have been doled out as indicated by the nitty gritty PED results got from the MOLVIB program. In present case, the determined harmonic wavenumbers of two premise 6-31G+(d) and 6-311G++(d,p) set looked at on account of the blend of electron relationship impacts and premise set inadequacies. The noticed FT-IR and FT-Raman spectra of the title particle are appeared in Figs. 5 and 6, separately. The noticed FT-IR, FT-Raman wavenumbers and determined wavenumbers utilizing thickness practical B3LYP strategies with two premise set alongside their relative forces, likely tasks of the compound are summed up in Table 2.

Ring Vibrations

The fragrant ring vibrational methods of title particle have been investigated dependent on the vibrational spectra of recently distributed vibrations of benzene atom is more useful in the distinguishing pieces of proof of the phenyl ring modes [23]. The ring extending vibrations are exceptionally noticeable, as the twofold bond is in formation with the ring, in the vibrational spectra of benzene and its subordinates [24]. The CC extending vibration happens in the area of 1650–1200 cm^{-1} . When all is said in done, the groups of variable force and are seen at 1625–1590, 1590–1575, 1540–1470, 1465–1430 and 1380–1280 cm^{-1} from the recurrence ranges given by Varsanyi [25] for the five groups in the locale. In the title particle, the peaks observed at 1637, 1350, 1275, 1125 and 950 cm^{-1} in FT-IR and at 1527, 1514, 1277, 944 and 805 cm^{-1} in FT-Raman are credited to CC extending vibration. The hypothetically scaled harmonic recurrence esteems at 1568, 1453, 1373, 1275, 1114, 988, and 773 cm^{-1} in B3LYP strategy. The frequencies saw in FT-IR range at 825 cm^{-1} have been assigned to ring breathing and comparing vibrations show up in FT-Raman range at 833 cm^{-1} shows great concurrence with perceptions. Typically, an in-plane deformity vibration is at higher frequencies than that the out-of-plane vibration [23]. The FT-IR band doled out at 950 and 944 cm^{-1} and 805 cm^{-1} in FT-Raman band are appointed to CCC in-plane twisting vibrations of 5H3HM1D. The anticipated CCC out of-plane twisting vibrations are additionally in acceptable concurrence with the deliberate qualities.

Methyl Group Vibrations

The title particle 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione viable has a solitary CH_3 bunch in first situation of the ring. For the tasks of CH_3 bunch frequencies, are can expect nine basics can be related to each CH_3 gathering, to be specific lopsided extending (CH_3ass), balanced extending (CH_3ss), in-plane bowing (CH_3ipb), out-of-plane bowing (CH_3opb), symmetric bowing (CH_3sb), in-plane shaking (CH_3ipr), out-of-plane shaking (CH_3opr) and contorting mode in CH_3 (CH_3twist). Methyl bunches are for the most part alluded as electron benefactor replacement in the fragrant ring framework. In fragrant mixtures, the CH_3 unbalanced extending vibrations happens at values more prominent than 3000 cm^{-1} and CH_3 symmetric extending vibrations happens at values only beneath than 3000 cm^{-1} [26]. The CH methyl bunch extending vibrations are by and large saw in the scope of 3000–2800 cm^{-1} [27]. The above outcomes from the unbalanced extending CH_3 mode in which the two CH obligations of the methyl bunch are broadening while the third one is contracting it is symmetric extending mode, in which all the three CH bonds expand and contract in stage. In the current case, the FT-IR and FT Raman band at 3068, 2954 and 3066 cm^{-1} address frequency mode. The

calculated asymmetric modes are 3060, 3057 and 2951 cm^{-1} at B3LYP methods good agreement with observed data. Two bending modes occur within a methyl group. At first, the symmetric bending vibration, involves the in-phase bending of CH bonds. The second the asymmetric bending vibration, involves out-of-phase bending of the CH bonds. For 5H3HM1D the values observed at 1524 cm^{-1} in FT-IR and 1432 cm^{-1} in FT-Raman spectrum are attributed to CH₃ in-plane bending vibrations.

CH Vibrations

Benzene ring usually display different groups in the area 3100–3000 cm^{-1} because of sweet-smelling CH extending vibration [28-29]. They are not influenced by the idea of the substituents. In the current examination, the band 3100 cm^{-1} are assigned to CH extending vibration in FT-IR and comparing FT-Raman vibration are attributed at 3432 cm^{-1} . The noticed wavenumbers of CH extending vibration are likewise in acceptable concurrence with the deliberate qualities and writing information [30]. The CH in-plane and out-of-plane bowing vibrations by and large lie in the district 1300–1000 cm^{-1} and 1000–675 cm^{-1} [31], separately. As per above writing information, the frail band saw in FT-Raman range at 1433 cm^{-1} are appointed to CH in-plane bowing vibration with minor commitment of CCC extending vibration. They show great concurrence with the hypothetically registered qualities at 1260 and 1185 cm^{-1} by B3LYP techniques. The medium and feeble groups saw at 900 and 888 cm^{-1} in the FT-IR and FT-Raman modes are assigned to CH out-of-plane bowing vibration of 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione.

CN Vibrations

The CN extending recurrence is a fairly difficult occupation since there are issues in recognizing these frequencies from different vibrations. The CN extending retention for sweet-smelling amines are distinguished in the locale 1382–1266 cm^{-1} [32]. In the current investigation, the CN extending vibrations are noticed distinctly at 1388 cm^{-1} in FT Raman spectra is acceptable concurrence with the trial esteems 1278 and 1275 cm^{-1} and processed qualities determined at 1385 cm^{-1} in B3LYP strategies with 6-31G+(d) and 6-311G++(d,p) premise set. Every one of the groups lie in the normal reach when contrasted with the writing [33].

CO Vibrations

Typically, the groups around 1300–1200 cm^{-1} are allocated to CO extending vibrations for subbed phenol [34]. In the current investigation, frail band at 1237 and 1250 cm^{-1} in FT-IR and FT-Raman range. The CO in-plane twisting vibrations are seen at 934 and 938 cm^{-1} in FT-IR and FT-Raman spectra. The determined out-of-plane twisting vibrations are figured at 1700, 1680, 1225 and 652 cm^{-1} by B3LYP strategies, separately.

NH Vibrations

The NH extending frequencies are seen in the locale at 3500 to 3300 cm^{-1} . [35] The NH extending mode was determined at 3499 cm^{-1} with 100% PED commitment. The wide pinnacle saw at 3525 cm^{-1} in FT-IR range compares to NH extending vibration. The NH in-plane twisting vibration was accounted for in the wavenumber locale of 1412 to 1415 cm^{-1} . The solid pinnacle was seen at 3440 cm^{-1} in FT-IR, and FT-Raman range relates to NH in-plane bowing mode.

Pyrrole Ring Vibrations

The heteroaromatic structure shows the CH extending frequencies in the wavenumber area of 3100 to 3000 cm^{-1} . The CH extending method of the pyrrole ring was determined as 3100 cm^{-1} with a PED estimation of 99%. An exceptionally frail FT-Raman top saw at 3078 cm^{-1} relates to the CH extending vibration of pyrrole ring. The CH in-plane twisting vibrations of pyrrole and its subordinators by and large happen in the locale of

1300 to 1000 cm^{-1} . [36] The CH in-plane bowing modes were determined as 1433 cm^{-1} . The comparing mode was seen at 1204 cm^{-1} in FT-IR range and at 1432, 1483 cm^{-1} in FT-Raman range. The CH out of plane bowing was determined at 857 cm^{-1} with a commitment of 75% in PED. The ring CC extending vibrational mode was determined as 1545 cm^{-1} . The CN extending vibrations by and large happen in the locale at 988 to 1275 cm^{-1} . [37] For the title atom, the C N extending vibration was determined as 1385 cm^{-1} . This mode was seen at 1350 cm^{-1} in FT-IR range and 1388 cm^{-1} in Raman range.

OH Vibrations

The OH extending frequencies are seen in the locale at 3550-3200 cm^{-1} . The OH extending mode was determined at 3432 cm^{-1} with 100% PED commitment. The peaks observed at 3193 cm^{-1} in FT-IR range compares to OH extending vibration.

Polarizability and Hyperpolarizability

The polarizability (α), hyperpolarizability (β) and electric dipole second (μ) for conformer C1 of the 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione are determined by limited field technique utilizing B3LYP strategies with 6-31G+(d) and 6-311G++(d,p) premise set and are introduced in Table 1. To figure all the electric dipole second and the principal hyperpolarizability tensor parts for a given framework will rely upon the decision of the Cartesian co-ordinate framework (x, y, z) = (0, 0, 0) was picked at own centre of mass of atom. The polarizability of this novel sub-atomic framework for $\alpha_{xx} = \alpha_{yy} = \alpha_{zz}$ is supposed to be isotropic. The polarizability is isotropic or same every which way for an atomic framework whose electron thickness is roundly balanced. In the event that the atom is entirely isotropic (P) and (E) will have same bearing and is then a straightforward scalar amount. The polarizability of this novel sub-atomic framework for which $\alpha_{xx} - \alpha_{yy} - \alpha_{zz}$ (P) will presently don't have a similar bearing as (E). The principal hyperpolarizability (β_{tot}) and related properties (α , β and $\Delta\alpha$) of 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione are determined and it depends on the limited field approach. Within the sight of an outside electric field (E), the energy of a framework is an element of the electric field. First hyperpolarizability is a third position component that can be depicted by a 3x3x3 lattice. The 27 parts of the 3D network can be diminished to 10 segments due to the Kleinman balance [38]. Clearly the lower part of the 3x3x3 lattices is tetrahedral. The segments of β are characterized as, the coefficients in the Taylor arrangement development of energy in an outer electric field. The outer electric field is powerless and homogeneous, this becomes:

$$E = E^0 - \frac{\mu_i F_i}{1!} - \frac{\alpha_{ij} F_i F_j}{2!} - \frac{\beta_{ijk} F_i F_j F_k}{3!} - \frac{\gamma_{ijkl} F_i F_j F_k F_l}{4!} + \dots$$

where E^0 is the energy of the unperturbed atoms, F_i is the field at the root and μ_i , α_{ij} , β_{ijk} and γ_{ijkl} are the parts of dipole second, polarizability and the hyperpolarizability, individually. The absolute static dipole second (μ), the mean polarizability (α), the anisotropy of the polarizability $\Delta\alpha$ and the mean first hyperpolarizability (β_{tot}), utilizing the x, y, z parts can be determined utilizing the accompanying conditions:

The absolute static dipole second is

$$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)$$

The isotropic polarizability is

$$\alpha = \frac{\alpha_{xx} + \alpha_{yy} + \alpha_{zz}}{3}$$

The polarizability anisotropy invariant is

$$\Delta\alpha = 2^{-\frac{1}{2}} [(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 + 6X_{xx}^2]$$

The normal hyperpolarizability

$$\beta_{tot} = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{1/2}$$

Where

$$\beta_x = (\beta_{xxx} + \beta_{xyy} + \beta_{xzz})$$

$$\beta_y = (\beta_{yyy} + \beta_{xxy} + \beta_{yzz})$$

$$\beta_z = (\beta_{zzz} + \beta_{xxz} + \beta_{yyz})$$

where α_{xx} , α_{yy} and α_{zz} are tensor components of polarizability. β_x , β_y and β_z are tensor segments of hyperpolarizability. Since the estimation of polarizability and hyper polarizability of the GAUSSIAN 09 yield are accounted for in nuclear units (a.u.), the determined qualities have been changed over into electrostatic units (e.s.u.) (1 a.u. = 8.639×10^{-33} e.s.u.). The all out sub-atomic dipole second, polarizability and first hyper polarizability are 1.6524 debye, 1.3982×10^{-30} e.s.u. what's more, 0.2012×10^{-30} e.s.u. in B3LYP/6-31G(d,p) and 1.6524 debye, 1.3982×10^{-30} e.s.u. furthermore, 0.2012×10^{-30} e.s.u. in 6-311G(d,p) techniques, separately.

Mulliken's Atomic Charge

In Mulliken's examination, a large portion of the cover populace is appointed to each contributing orbital, giving the all-out populace of each nuclear orbital. Adding in general the nuclear orbitals on a particular molecule gives as the gross nuclear populace. The charge appropriations determined by the Mulliken [39]. The charge dispersion on the particle impacts the vibrational spectra [40]. The estimations of the Mulliken's nuclear charges of an every molecule for conformer C1 of the title compound were additionally gotten with the assistance of B3LYP levels of hypothesis fusing 6-31G+(d) and 6-311G++(d,p) premise set. The Mulliken's nuclear charges on every molecule of the title compound the graphical portrayal is appeared in Fig. 7.

Frontier Molecular Orbital Studies

The Frontier Molecular Orbital (FMO), for example, most elevated involved sub-atomic orbital (HOMO) and least vacant sub-atomic orbital (LUMO) has urgent impact in the synthetic dependability of the particle [41]. The HOMO addresses, capacity to give an electron and LUMO addresses, capacity of acknowledge an electron. The energy hole among HOMO and LUMO additionally decides the compound reactivity, optical polarizability, substance hardness and non-abrasiveness of a particle. An atom with a little boondocks orbital hole is polarizable and is related with a high substance reactivity, low motor strength and is likewise named as delicate particle [42]. As per the outcomes, the 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione contains 61 involved atomic orbitals and 177 vacant sub-atomic orbitals. The HOMO and LUMO energies determined at B3LYP techniques with 6-31G+(d) and 6-311G++(d,p) premise set for conformer C1 are introduced in Table 3. The HOMO, HOMO1 pictures of C1 conformer and their orbital energies are determined by determined by B3LYP with 6-31G+(d) and 6-311G++(d,p) techniques separately. The positive stage is red and negative one. It is clear shows that the isodensity plots for the HOMO and LUMO are all around confined and the intramolecular communications generally happened inside the ring. In the HOMO surface, the holding p orbital's spreading preposterous carbon particles are useful to hold the atom together. It merits referencing here that the sub-atomic orbital flaps which situated on the molecules N₁₆, N₁₇, O₂₂, O₂₄ and O₂₅ of the HOMO surface is a non-holding orbital. Subsequently, the electrons in oxygen molecule act like a solitary pair of electrons in a Lewis structure. The energy hole among HOMO and LUMO clarifies the terminal charge move cooperation inside the particle, which impact the natural action of an atom. On account of 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione the littlest energy hole of $\Delta E_1 = 0.0520$ eV are

recognized between the HOMO and LUMO with the assistance of B3LYP 6-31G+(d) and 6-311G++(d,p) techniques. The atomic measure of ionization potential (I), electron fondness (A), electronic substance potential (μ), electronegativity (χ), worldwide hardness (η), worldwide delicateness (ν) and worldwide electrophilicity (ω) of the particle by DFT technique (B3LYP levels) were introduced in Table 3 for the conformer C1. In straightforward particle orbital hypothesis draws near, the HOMO energy (EHOMO) is identified with the ionization potential (IP) by Koopmans' hypothesis and LUMO energy (ELUMO) has been utilized to assess the electron liking (EA) [43].

$$I = -E_{HOMO}$$

$$A = -E_{LUMO}$$

The normal estimation of the HOMO and LUMO energies is identified with the electronegativity (χ) characterized by Mulliken [44].

$$\chi = \frac{(I + A)}{2}$$

Also, the HOMO and LUMO energy is identified with the hardness (η) and non-abrasiveness (ν) [45–47].

$$\eta = \frac{(I - A)}{2}$$

$$\nu = 1/\eta$$

$$\sigma = \frac{1}{\eta}$$

Parr et al. [48] characterized worldwide electrophilicity (ω).

$$\omega = \left(\frac{\mu^2}{2\eta} \right)$$

where μ is the compound potential takes the normal estimation of IP and EA [49].

$$\mu = -(IP+EA)/2$$

Molecular Electrostatic Potential (MEP)

Atomic electrostatic potential (MEP) at a point in space around a particle gives data about the net electrostatic impact created by then by absolute charge dissemination (electron and proton) of the atom [50]. The connection between the positive charge and some point in the particle is supposed to be alluring if the fact of the matter is negative charged; unpleasant on the off chance that it is positive charged, and the strength of cooperation rely upon the greatness of the charge. It is not difficult to show this guide utilizing the shades of the rainbow from red to blue. Red is the negative end (electron – rich) and blue is the positive end (electron – poor). For the frameworks considered the MEP esteems are determined as portrayed beforehand, utilizing the condition [51].

$$V(r) = \sum \frac{Z_A}{|R_A - r|} - \int \frac{\rho(r')}{|r' - r|} dr$$

where the summation runs over every one of the cores A_n in the compound and polarization and revamping impacts are disregarded. Z_A is the charge of the core A, situated at R_A and $\rho(r')$ is the electron thickness capacity of the compound. The MEP surface is plotted over streamlined math of the conformer C1 at B3LYP strategies with 6-31G+(d) and 6-311G++(d,p) premise set. Fig. 8 shows electrostatic possible counter guide of 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione alongside the fitting point charges to the electrostatic potential, the electron thickness isosurface being 0.002 a.u. the electrostatic potential guide shows that the molecules O_{22} , O_{24} and O_{25} are the most electronegative particle in B3LYP strategies for 5-Aziridinyl-3-

hydroxymethyl-1-methylindole-4,7-dione. The determined point charge relating particles C₇, H₉, C₁₀, C₁₁, H₁₂, H₁₃, C₁₈, C₂₆, H₂₇ And H₂₉ in the conformer C1 which is the most electropositive molecule in the 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione, individually.

V.CONCLUSION

The FT-IR and FT-Raman spectra of 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione, were completed interestingly. A total vibrational and sub-atomic underlying investigation has been done dependent on the quantum mechanical methodology by DFT computation. The balance mathematical and harmonic frequencies were resolved and dissected for the most steady conformer C1 utilizing B3LYP levels with 6-31G+(d) and 6-311G++(d,p) premise set. In this way, the tasks with sensible deviation from the two-premise esteem appear to be right. The examination shows the scaled computations are incredible methodology for understanding the vibrational spectra of the title particle. The determined HOMO and LUMO energy hole (0.0520eV) are affirm the presence of charge move inside the C1 conformer of the atom. The HOMO and LUMO energies can be utilized to assess the ionization potential, electron liking, electronegativity, electrophilicity file, worldwide hardness, non-abrasiveness and compound capability of the atom. The anticipated sub-atomic electrostatic potential demonstrates that this particle has a few potential destinations for electrophilic assault in which V(r) estimations give bits of knowledge into the request for presence. The high negative locales are related inside the atom O₂₂, O₂₄ and O₂₅. In this manner, it will be the favoured electrophilic destinations and positive locales of molecules C₇, H₉, C₁₀, C₁₁, H₁₂, H₁₃, C₁₈, C₂₆, H₂₇ And H₂₉ are favoured nucleophilic destinations.

Table 1: Optimized geometrical parameters of 5-aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione by B3LYP/6-31+G(d) and B3LYP/6-311++G(d,p) methods.

Para Meters	Bond lengths (Å)		Parameters	Bond angles (degrees)		Parameters	Dihedral angles (degrees)	
	B3LYP			B3LYP			B3LYP	
	6-31+G(d)	6-311++G(d,p)		6-31+G(d)	6-311++G(d,p)		6-31+G(d)	6-311++G(d,p)
C ₁ -C ₂	1.39	1.39	C ₂ -C ₁ -C ₆	121.37	121.37	C ₆ -C ₁ -C ₂ -C ₃	-0.35	-0.35
C ₁ -C ₆	1.45	1.45	C ₂ -C ₁ -C ₇	107.83	107.83	C ₆ -C ₁ -C ₂ -N ₁₇	-179.81	-179.81
C ₁ -C ₇	1.42	1.42	C ₆ -C ₁ -C ₇	130.78	130.78	C ₇ -C ₁ -C ₂ -C ₃	179.46	179.46
C ₂ -C ₃	1.46	1.46	C ₁ -C ₂ -C ₃	123.81	123.81	C ₇ -C ₁ -C ₂ -N ₁₇	0.004	0.004
C ₂ -N ₁₇	1.36	1.36	C ₁ -C ₂ -N ₁₇	108.08	108.08	C ₂ -C ₁ -C ₆ -C ₅	-0.62	-0.62
C ₃ -C ₄	1.46	1.46	C ₃ -C ₂ -N ₁₇	128.10	128.10	C ₂ -C ₁ -C ₆ -O ₂₅	178.88	178.88
C ₃ -O ₂₄	1.23	1.23	C ₂ -C ₃ -C ₄	114.62	114.62	C ₇ -C ₁ -C ₆ -C ₅	179.59	179.59
C ₄ -C ₅	1.36	1.36	C ₂ -C ₃ -O ₂₄	123.17	123.17	C ₇ -C ₁ -C ₆ -O ₂₅	-0.89	-0.89
C ₄ -H ₈	1.08	1.08	C ₄ -C ₃ -O ₂₄	122.20	122.20	C ₂ -C ₁ -C ₇ -C ₁₈	0.04	0.04
C ₅ -C ₆	1.52	1.52	C ₃ -C ₄ -C ₅	123.45	123.45	C ₂ -C ₁ -C ₇ -C ₁₉	179.86	179.86
C ₅ -N ₁₆	1.37	1.37	C ₃ -C ₄ -H ₈	115.61	115.61	C ₆ -C ₁ -C ₇ -C ₁₈	179.84	179.84
C ₆ -O ₂₅	1.22	1.22	C ₅ -C ₄ -H ₈	120.91	120.91	C ₆ -C ₁ -C ₇ -C ₁₉	-0.33	-0.33
C ₇ -C ₁₈	1.38	1.38	C ₄ -C ₅ -C ₆	121.43	121.43	C ₁ -C ₂ -C ₃ -C ₄	0.63	0.63

C ₇ -C ₁₉	1.49	1.49	C ₄ -C ₅ -N ₁₆	123.16	123.16	C ₁ -C ₂ -C ₃ -O ₂₄	-179.08	-179.08
H ₉ -C ₁₈	1.07	1.07	C ₆ -C ₅ -N ₁₆	115.22	115.22	N ₁₇ -C ₂ -C ₃ -C ₄	179.98	179.98
C ₁₀ -C ₁₁	1.50	1.50	C ₁ -C ₆ -C ₅	115.27	115.27	N ₁₇ -C ₂ -C ₃ -O ₂₄	0.27	0.27
C ₁₀ -H ₁₂	1.09	1.09	C ₁ -C ₆ -O ₂₅	123.83	123.83	C ₁ -C ₂ -N ₁₇ -C ₁₈	-0.05	-0.05
C ₁₀ -H ₁₃	1.08	1.08	C ₅ -C ₆ -O ₂₅	120.87	120.87	C ₁ -C ₂ -N ₁₇ -C ₂₆	179.90	179.90
C ₁₀ -N ₁₆	1.45	1.45	C ₁ -C ₇ -C ₁₈	105.83	105.83	C ₃ -C ₂ -N ₁₇ -C ₁₈	-179.48	-179.48
C ₁₁ -H ₁₄	1.08	1.08	C ₁ -C ₇ -C ₁₉	127.50	127.50	C ₃ -C ₂ -N ₁₇ -C ₂₆	0.47	0.47
C ₁₁ -H ₁₅	1.08	1.08	C ₁₈ -C ₇ -C ₁₉	126.66	126.66	C ₂ -C ₃ -C ₄ -C ₅	0.15	0.15
C ₁₁ -N ₁₆	1.45	1.45	C ₁₁ -C ₁₀ -H ₁₂	117.74	117.74	C ₂ -C ₃ -C ₄ -H ₈	178.69	178.69
N ₁₇ -C ₁₈	1.37	1.37	C ₁₁ -C ₁₀ -H ₁₃	120.13	120.13	O ₂₄ -C ₃ -C ₄ -C ₅	179.87	179.87
N ₁₇ -C ₂₆	1.46	1.46	H ₁₂ -C ₁₀ -H ₁₃	115.29	115.29	O ₂₄ -C ₃ -C ₄ -H ₈	-1.57	-1.57
C ₁₉ -H ₂₀	1.09	1.09	H ₁₂ -C ₁₀ -N ₁₆	117.29	117.29	C ₃ -C ₄ -C ₅ -C ₆	-1.16	-1.16
C ₁₉ -H ₂₁	1.09	1.09	H ₁₃ -C ₁₀ -N ₁₆	115.69	115.69	C ₃ -C ₄ -C ₅ -N ₁₆	173.89	173.89
C ₁₉ -O ₂₂	1.43	1.43	C ₁₀ -C ₁₁ -H ₁₄	120.45	120.45	H ₈ -C ₄ -C ₅ -C ₆	-179.64	-179.64
O ₂₂ -H ₂₃	0.96	0.96	C ₁₀ -C ₁₁ -H ₁₅	117.62	117.62	H ₈ -C ₄ -C ₅ -N ₁₆	-4.58	-4.58
C ₂₆ -H ₂₇	1.09	1.09	H ₁₄ -C ₁₁ -H ₁₅	115.20	115.20	C ₄ -C ₅ -C ₆ -C ₁	1.38	1.38
C ₂₆ -H ₂₈	1.09	1.09	H ₁₄ -C ₁₁ -N ₁₆	115.43	115.43	C ₄ -C ₅ -C ₆ -O ₂₅	-178.14	-178.14
C ₂₆ -H ₂₉	1.09	1.09	H ₁₅ -C ₁₁ -N ₁₆	117.51	117.51	N ₁₆ -C ₅ -C ₆ -C ₁	-174.04	-174.04
			C ₅ -N ₁₆ -C ₁₀	125.08	125.08	N ₁₆ -C ₅ -C ₆ -O ₂₅	6.42	6.42
			C ₅ -N ₁₆ -C ₁₁	125.65	125.65	C ₄ -C ₅ -N ₁₆ -C ₁₀	43.85	43.85
			C ₂ -N ₁₇ -C ₁₈	108.59	108.59	C ₄ -C ₅ -N ₁₆ -C ₁₁	122.70	122.70
			C ₂ -N ₁₇ -C ₂₆	126.64	126.64	C ₆ -C ₅ -N ₁₆ -C ₁₀	-140.79	-140.79
			C ₁₈ -N ₁₇ -C ₂₆	124.75	124.75	C ₆ -C ₅ -N ₁₆ -C ₁₁	-61.95	-61.95
			C ₇ -C ₁₈ -H ₉	129.34	129.34	C ₁ -C ₇ -C ₁₈ -H ₉	179.74	179.74
			C ₇ -C ₁₈ -N ₁₇	109.65	109.65	C ₁ -C ₇ -C ₁₈ -N ₁₇	-0.07	-0.07
			H ₉ -C ₁₈ -N ₁₇	120.99	120.99	C ₁₉ -C ₇ -C ₁₈ -H ₉	-0.07	-0.07
			C ₇ -C ₁₉ -H ₂₀	109.94	109.94	C ₁₉ -C ₇ -C ₁₈ -N ₁₇	-179.89	-179.89
			C ₇ -C ₁₉ -H ₂₁	109.98	109.98	C ₁ -C ₇ -C ₁₉ -H ₂₀	-58.48	-58.48
			C ₇ -C ₁₉ -O ₂₂	108.23	108.23	C ₁ -C ₇ -C ₁₉ -H ₂₁	58.96	58.96
			H ₂₀ -C ₁₉ -H ₂₁	106.90	106.90	C ₁ -C ₇ -C ₁₉ -O ₂₂	-179.77	-179.77
			H ₂₀ -C ₁₉ -O ₂₂	110.90	110.90	C ₁₈ -C ₇ -C ₁₉ -H ₂₀	121.29	121.29
			H ₂₁ -C ₁₉ -O ₂₂	110.86	110.86	C ₁₈ -C ₇ -C ₁₉ -H ₂₁	-121.24	-121.24
			C ₁₉ -O ₂₂ -H ₂₃	108.63	108.63	C ₁₈ -C ₇ -C ₁₉ -O ₂₂	0.0063	0.0063
			N ₁₇ -C ₂₆ -H ₂₇	110.35	110.35	H ₁₂ -C ₁₀ -C ₁₁ -H ₁₄	-150.21	-150.21
			N ₁₇ -C ₂₆ -H ₂₈	110.36	110.36	H ₁₂ -C ₁₀ -C ₁₁ -H ₁₅	-0.30	-0.30
			N ₁₇ -C ₂₆ -H ₂₉	108.07	108.07	H ₁₃ -C ₁₀ -C ₁₁ -H ₁₄	-0.49	-0.49
			H ₂₇ -C ₂₆ -H ₂₈	108.25	108.25	H ₁₃ -C ₁₀ -C ₁₁ -H ₁₅	149.40	149.40
			H ₂₇ -C ₂₆ -H ₂₉	109.91	109.91	H ₁₂ -C ₁₀ -N ₁₆ -C ₅	8.40	8.40
			H ₂₈ -C ₂₆ -H ₂₉	109.88	109.88	H ₁₃ -C ₁₀ -N ₁₆ -C ₅	-133.01	-133.01

						H ₁₄ -C ₁₁ -N ₁₆ -C ₅	133.38	133.38
						H ₁₅ -C ₁₁ -N ₁₆ -C ₅	-7.82	-7.82
						C ₂ -N ₁₇ -C ₁₈ -C ₇	0.08	0.08
						C ₂ -N ₁₇ -C ₁₈ -H ₉	-179.75	-179.75
						C ₂₆ -N ₁₇ -C ₁₈ -C ₇	-179.88	-179.88
						C ₂₆ -N ₁₇ -C ₁₈ -H ₉	0.27	0.27
						C ₂ -N ₁₇ -C ₂₆ -H ₂₇	-59.77	-59.77
						C ₂ -N ₁₇ -C ₂₆ -H ₂₈	59.83	59.83
						C ₂ -N ₁₇ -C ₂₆ -H ₂₉	180.01	180.01
						C ₁₈ -N ₁₇ -C ₂₆ -H ₂₇	120.18	120.18
						C ₁₈ -N ₁₇ -C ₂₆ -H ₂₈	-120.21	-120.21
						C ₁₈ -N ₁₇ -C ₂₆ -H ₂₉	-0.029	-0.029
						C ₇ -C ₁₉ -O ₂₂ -H ₂₃	179.47	179.47
						H ₂₀ -C ₁₉ -O ₂₂ -H ₂₃	58.78	58.78
						H ₂₁ -C ₁₉ -O ₂₂ -H ₂₃	-59.81	-59.81

Table 2: Vibrational assignments of FT-IR and FT-Raman peaks along the theoretically computed wave numbers, IR (I_{IR}) and Raman intensity (I_{Raman}) and the percentage of potential energy distribution of 5-aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione

S. No	Observed wave number (cm ⁻¹)		B3LYP/6-31+G(d) / B3LYP/6-311++G(d,p)				Assignments with % of PED
	FT- IR	FT-Raman	Calculated wave number (cm ⁻¹)		I_{IR}	I_{Raman}	
			Un scaled	Scaled			
1	3525		3773.02	3440	398.76	399.96	v NH(98)
2	3432	3432	3292.06	3193	315.29	212.57	γ C-H (97)
3	3100		3226.02	3060	297.46	197.26	β C-H(96)
4		3078	3206.05	3075	206.52	181.12	vCH (99)
5	3053		3203.77	3057	197.77	177.48	vCH(100)
6			3167.06	3059	161.39	172.97	v CH(str)
7	3025		3156.20	2951	153.17	144.71	v CH(98)
8			3136.98	2989	115.99	141.61	CH ₃ ass(98),
9	2954		3118.18	2959	92.85	127.95	CH ₃ ass(97)
10	2920		3081.44	2924	88.42	107.45	CH ₃ ass(94)
11			3039.99	2728	70.17	92.98	CH ₃ ss(99)
12		2716	3015.55	2720	67.02	87.03	CH ₃ ss(97)
13	1750	1777	1720.32	1700	66.48	72.98	v C=O(97)
14		1694	1690.83	1680	58.06	67.61	v C=O(81)

15	1637	1527	1632.24	1568	52.17	64.25	v C=C str(52)
16	1524		1598.13	1527	47.18	62.72	CH ₃ ipb(61)
17		1483	1541.53	1484	45.69	62.22	CH ₃ ipb(97)
18		1514	1539.69	1453	39.74	58.43	v C=C str(78)
19			1525.42	1389	37.32	56.46	ω C-C-N(77),
20	1432		1520.81	1433	37.06	45.18	CH ₃ ipb(93)
21	1420		1509.32	1422	32.64	43.38	CH ₃ ipb(86)
22			1508.47	1407	30.67	37.15	vCCC (79)
23		1526	1499.46	1396	30.50	34.88	CH ₃ opb(89)
24		1388	1467.53	1385	29.51	33.65	v C-N(91)
25			1451.12	1366	28.15	23.92	CH ₃ sb(84)
26			1440.52	1380	27.77	23.55	β CH bend(61)
27			1422.00	1375	25.24	23.18	vC-H(98)
28	1350		1387.78	1373	25.07	22.29	vC=C(52),
29			1342.08	1328	24.33	20.56	v CH rock,
30			1305.91	1314	22.63	19.35	v C-N str(74),
31	1275	1277	1253.07	1275	21.88	18.69	σ C-C str (7)
32		1182	1244.28	1185	20.18	16.55	βCH(82),
33	1225		1231.91	1260	19.48	13.58	v CH rock
34	1175		1191.15	1225	18.84	13.41	v C-O(50)
35	1125		1183.02	1128	17.18	13.38	CH ₃ ipr(97)
36	1057		1175.13	1060	16.68	13.25	CH ₃ ipr(77),
37	1034		1160.49	1036	12.48	11.49	CH ₃ opr(98)
38		1194	1153.93	1170	12.33	11.43	γCHipb
39			1139.68	1151	12.22	10.97	γ CH ipb
40		1166	1132.63	1136	11.24	9.80	γ CH ipb(14)
41	1125		1112.63	1114	10.35	9.14	v C-C(62)
42			1078.62	1094	10.11	8.57	v C-C str(21)
43			1051.68	954	9.58	8.25	CH ₃ opr(98)
44			1047.31	948	8.17	7.22	CH ₃ opr(98),
45			1038.20	1094	7.22	6.96	v C-C str(21),
46			979.85	1049	6.90	6.69	γ CH rock(69),
47	950	944	962.18	988	6.69	6.19	v C-C(62)
48	900		896.22	930	6.60	5.65	β CH rock(50)
49		888	867.93	884	6.15	5.51	β C-H(15)
50			835.34	815	5.97	4.68	η(41)
51	825	833	810.21	857	5.82	4.11	v CH opw (93)
52		805	803.13	773	5.24	3.63	v C-C (92)
53			780.59	768	4.52	3.45	v CH rock (90),

54	750	749	734.92	748	3.83	3.08	v CH rock(82)
55			733.12	748	2.99	3.03	β CH opw(80),
56			690.23	748	2.46	2.42	v P-CH ₂ (72)
57			636.11	704	2.42	2.35	v N-H(57)
58		666	629.51	670	2.40	2.18	γ ring def(54)
59	595		617.69	610	2.22	2.13	η (13)
60		650	592.60	652	2.11	1.94	v C-O(45)
61			500.69	492	2.11	1.63	v ring str(91)
62			477.75	489	2.05	1.57	v C-C-N (82)
63			433.78	461	2.05	1.40	γ ring def (76)
64		416	407.59	442	1.92	1.14	β ring def(74)
65			376.62	354	1.75	1.04	v NH rock(50)
66			350.02	335	1.68	1.02	v N-H(52),
67	300		310.99	317	1.65	0.97	ω N-H ₂ (14
68		289	305.12	288	1.42	0.96	β C-CH ₃ (89)
69			251.79	240	1.30	0.89	CH ₃ twist(82)
70			244.02	233	1.08	0.77	γ ring def(58)
71			226.75	221	1.07	0.74	γ C-H, β C-N(64)
72			220.91	210	0.92	0.73	γ C-CH ₃ (82)
73			173.61	173	0.71	0.71	CH ₃ twist(97)
74		166	158.76	176	0.61	0.67	v ring bend(52)
75			133.33	132	0.60	0.64	CH ₃ twist(92)
76			119.66	76	0.58	0.54	γ C-OCH ₃ (22)
77		111	103.54	117	0.44	0.49	β C-C-C(54)
78			86.95	69	0.36	0.35	γ C-CH ₃ (62),
79			79.57	69	0.27	0.34	v C-O(17),
80			64.80	52	0.07	0.30	γ C-CH ₃ (69)
81			47.10	52	0.05	0.10	γ C-CH ₃ (69)

ass-asym. stretching, ss-symstretching, ipb-in-plane-bending, opb-out-of-planebending, sb-sym.bending, ipr-in-plane rocking, opr-out-of-plane rocking, sciss-scissoring, rock-rocking, wagg-wagging, twist-twisting. Assignments: v-stretching, β -in-plane bending, γ -out-of-plane bending

Table 3: Comparison of HOMO, LUMO energy gaps and related molecular properties of 5-aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione at B3LYP/631G+(d) and B3LYP/6311G++(d,p) level of theory

Molecular Properties	Energy (a.u)	Energy gap (eV)	Ionization Potential (I _p)	Electron Affinity (E _A)	Global Hardness (η)	Electro negativity (χ)	Global Softness (ν)	Chemical Potential (μ)	Global Electrop hilicity (ω)
HOMO	- 0.3087	0.0520	0.3087	0.2566	0.0260	0.2826	38.461	-0.2826	1.519
LUMO	-0.2566								
HOMO-1	-0.3200	0.1795	0.3200	0.1405	0.0897	0.2302	11.148	-0.2302	0.2948
LUMO+1	-0.1405								

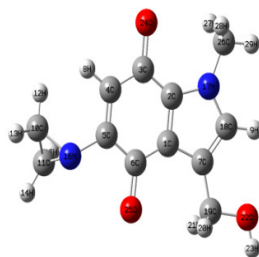


Fig.1.Molecular Geometry Structure of 5-aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione

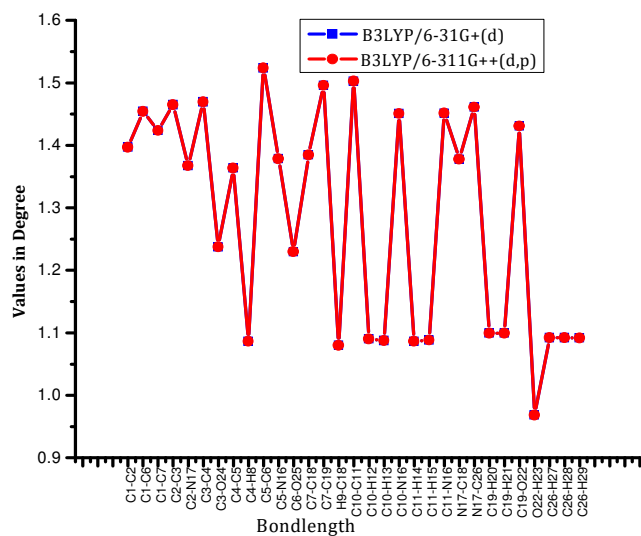


Fig.2. Bond Length Difference Between Theoretical B3LYP/6311G++(d,p) and B3LYP/631G+(d) 5-Aziridinyl-3-Hydroxymethyl-1-Methylindole-4,7-dione

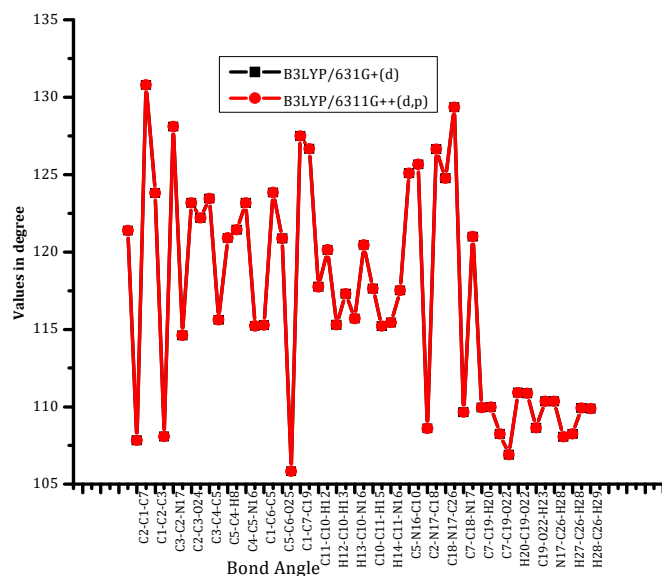


Fig.3. Bond Angle Difference Between Theoretical B3LYP/6311G++(d,p) and B3LYP/631G+(d) 5-Aziridinyl-3-Hydroxymethyl-1-Methylindole-4,7-dione

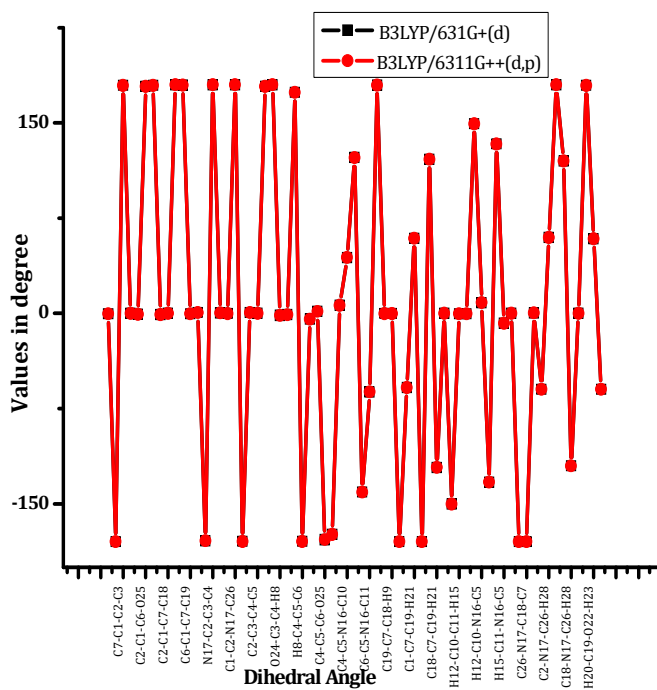


Fig.4. Dihedral Angle Difference Between Theoretical B3LYP/6311G++(d,p) and B3LYP/631G+(d) 5-Aziridinyl-3-Hydroxymethyl-1-Methylindole-4,7-dione

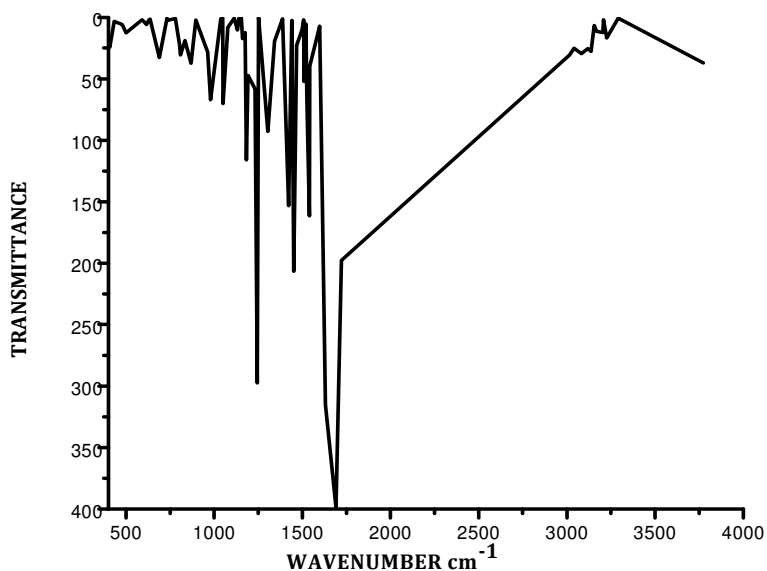


Fig.5. Observed FT-IR of 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione

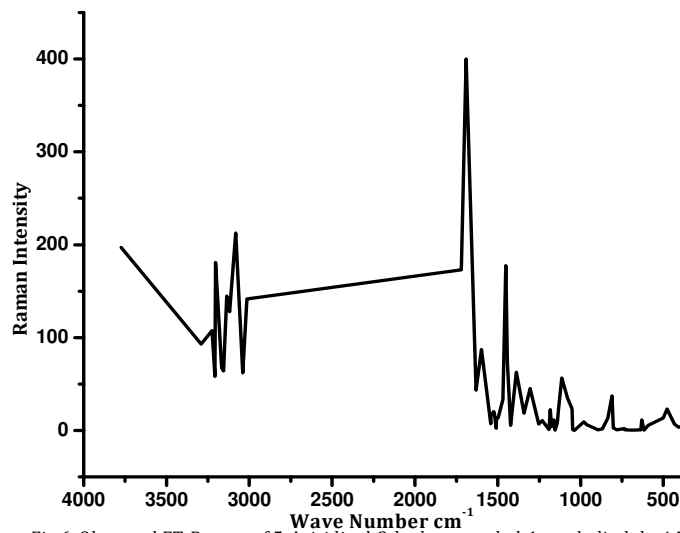


Fig.6. Observed FT-Raman of 5-Aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione

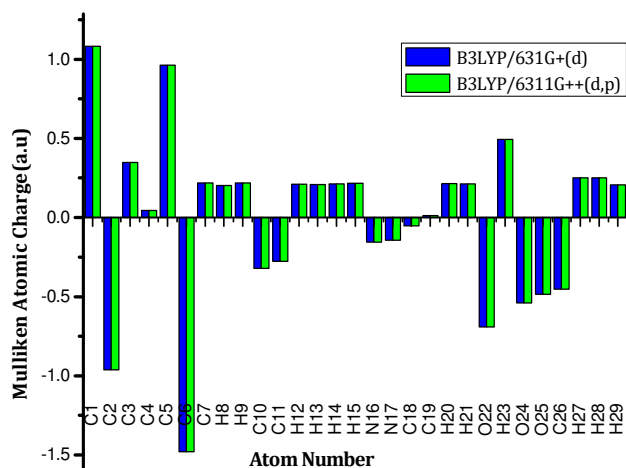


Fig.7 Mulliken population analysis chart of 5-aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione B3LYP/631G+(d) and B3LYP/6311G++(d,p) methods

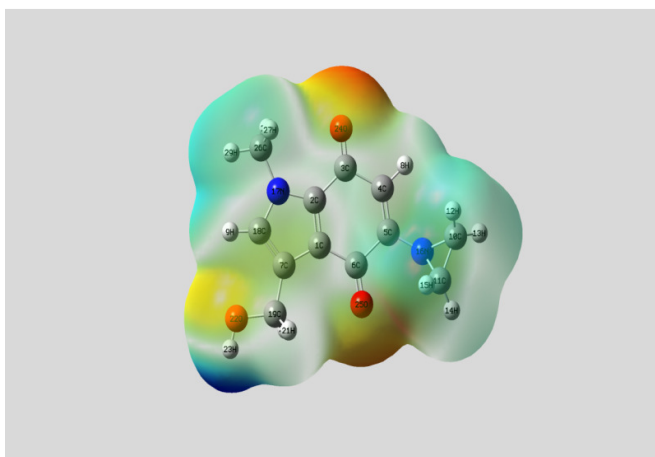


Fig.8. Molecular Electrostatic Potential of 5-aziridinyl-3-hydroxymethyl-1-methylindole-4,7-dione

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