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GRAPHICAL ABSTRACT



Study of molecular structure, chemical reactivity and first hyperpolarizability of a newly synthesized N-(4-oxo-2-phenylquinazolin-3(4H)-yl)-1H-indole-2-carboxamide using spectral analysis

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Abstract

A series of novel Quinazolinone derivatives were synthesized and characterized by various spectroscopic techniques. The nature of reactants and products of chemical reactions has been determined using thermodynamic parameters (H, G, S). The TD–DFT calculation of the compound shows that electronic excitations is $n\rightarrow\pi^*$ in nature and compounds having intramolecular hydrogen bonding is obvious in ¹H NMR, ¹³C NMR, FT–IR measurements and ESP map. In ¹H NMR signal of the indolic NH protons appears at 7.26 ppm shows that intramolecular hydrogen is present in compounds. The vibrational analysis designates the presence of intramolecular hydrogen bonding N12–H34…O21 shows in lowering of NH and CO stretching vibrations frequency. The local reactivity descriptors Fukui functions (f_k^+ , f_k^-), local softness's (s_k^+ , s_k^-) and electrophilicity indices (ω_k^+ , ω_k^-) determine the reactive sites within molecule. The computed first hyperpolarizability (β_0) found to be $10.2254 \times 10^{-30}esu$ indicating that the compound is non–linear optical (NLO) material.

Keywords: Quinazolinone, MESP, NLO analysis, chemical reactivity, first hyperpolarizability **Introduction**

One of the major problems facing humanity today in the context of life threatening disease such as microbial infections, protozoan Leishmaniasis [1], HIV/AIDS Co infections [2], Quinazoline derivatives, one of the most active classes of compounds possessing a wide spectrum of biological properties, for example, antitumor[3-5], anti-inflammatory[6,7], anticonvulsant [8] ,antioxidants [9], analgesic [10,11] for this reason, total synthesis of natural occurring quinazolinones e.g. Vasicinones [12,13] Fumiquinazolinones, Luotonins[14] Circumdatin[15] and Asperlicin[16] have earlier been reported. Quinazolinone have ability to reduce the C=O and C=N group by transfer of hydrogenation and have strong coordinating complex towards different metal ions Rh, Pt, Ir, Pd, Os and Ru [17].

Thus we synthesized compounds that related to the natural occurring quinazolinones and screened them for their Antimicrobial [18,19] and Antileishmanial [20] activity, the compounds were found promising results with a number 3-aminoquinazolinones with a known structures against microorganisms, therefore, we aim at this work is to be synthesis of some novel quinazolinone derivatives and to search for their antimicrobial potentialities. On methylation of 2- carboxylic indole of compound 1 by the reaction of methanol and sulphuric acid was used as a acid catalyst to form Methyl-2-indole carboxylate of compound **A**, further was reacted with hydrazine hydrate with ethanol, furnished 2-carbohydrazide indole of compound **2**. The compound **1** was reacted with compound **2** ethanol used as solvent and heated at 75° C for 3-6 hours to afford the targeted

compounds 3. A series of Quinazoline derivatives were screened for their antimicrobial, antileishmanial activity and characterized by spectroscopic techniques.

In observation of above applications of quinazolinone containing of compound **3** has synthesized and characterized by ¹H NMR, UV–Visible, FT-IR and Mass spectroscopic techniques. The geometry of compound **3** was optimized and harmonic vibrational frequencies were calculated by DFT/B3LYP level and using 6-31 G(d, p) basis set. The ¹H-NMR chemical shifts were calculated by GIAO method using same basis set. The results obtained theoretically compared with the experimental observations. The ¹H-NMR chemical shifts and vibrational analysis showed the existence of intramolecular H-bonding. It is also predicts the transition between HOMO-LUMO in compound 5 by using TD-DFT approach. Quantum chemical calculations are responsible for the determination of thermodynamic parameters such as enthalpy (H), entropy (S) and Gibb's free energy (G) and also predict feasibility of reactions. Molecular Electrostatic Potential surface (MEPS) investigation along with calculation of first hyperpolarizability (β_{0} evaluates the NLO properties of the compound. The global reactivity descriptors and local reactivity descriptor like Fukui functions have been calculated to elaborate various characteristic properties of the compound **3**.

Experimental Protocol:

All the reactions were monitored by thin layer chromatography over silica gel-G and basic alumina coated TLC plates and TLC was also performed using silica gel 60 F254 plates. The spot on TLC plates were developed by iodine vapours. The melting points were recorded on an electrically heated melting point apparatus and are uncorrected. IR spectra were recorded on Beckman Aculab-10, Perkin Elmer 881 and FT IR 8210 PC, Shimadzu spectrophotometers either on KBr discs or in neat and values are expressed in cm⁻¹. Nuclear Magnetic Resonance (NMR) spectra were recorded on either Bruker Advance DRX-300 MHz or Bruker DRX 200 FT spectrometers using TMS (0.0ppm) as an internal reference. Chemical shifts (δ in ppm) were reported relative to solvent peak (CHCl₃ in CDCl₃ at 7.23 ppm and DMSO in DMSO-d₆ at 2.49 ppm) or TMS. Signals were designated as follows: s, singlet; bs, broad singlet; d, doublet; dd, double doublet; t, triplet; m, multiplet and q, quartet. FAB mass spectra were recorded on JEOL SX 102/DA 6000 mass spectrometer using Argon/Xenon (6 KV, 10mA) as the FAB gas. EI mass spectra were recorded on JEOL JMS-D-300 spectrometer with ionization potential of 70 eV and ES mass on Quantro-II, micro mass.

Synthesis of Indole-2-methyl carboxylate (A)

On methylation of indole -2-carboxylic acid with methanol and sulphuric acid was added as acid catalyst. The reaction mixture was stirred at room temperature for 8-10hrs. After completion of reaction (Monitored by TLC), the solvent was evaporated on water bath the crud product obtained. It was purified by a column chromatography in a mixture of hexane and ethyl acetate (3:1). The solid crystalline compound obtained in good yield 65%.

Synthesis of Indole-2-carbohydrazide (2)

A mixture of methyl indole-2-carboxylate **A** (0.01 mole) and hydrazine hydrate (.01mole) in absolute ethanol, (30ml) was heated under reflux 5-7 hrs. After completion of reaction (Monitored by TLC) The reaction mixture was cooled at room temperature, precipitated solid was recrystallized in absolute ethanol. The crystalline compound Indole-2-carbohydrazide (**2**) was obtained in good yield (68%)

Synthesis of N-(4-oxo-2-phenylquinazolin-3(4H)-yl)-1H-indole-2carboxamide (compounds 3):

2-Phenyl-3,1-benzoxazin-4-(4H)-one (1) (0.5mole) was treated with Indole-2-carbohydrazide (2) equimolar proportion of (0.5 mol) using ethanol (25 ml) as a solvent the resulting the reaction mixture was refluxed for -4- 6 hrs., after completion of the reaction was (Monitoring by TLC), the excess of solvent was distilled off on rota vapour and the resulting solid obtained was dried and recrystallized by rectified sprit, affording the corresponding compounds (3) as colourless crystalline solid in good yields(70%).

IR (KBr Solid), 3399 NH, 3021 (CH), 1959 (C=0), 1616 (C=C), 1403 (C=N), 1316 (C=C), 1059 (C-O enol group); ¹H NMR (300MHz, CDCl₃): δ 7.26 (2NH, bs), 7.53-7.60 (m, 5H), 7.48 (s, 1H), 7.69 (d, J = 8.01 Hz, 2H), 7.80 (t, J = 9.00Hz, 2H), 7.83 (t, J = 7.1 Hz, 2H), 8.23 (d, J = 7.8 Hz, 2H), 8.3 (dd, J = 7.2Hz, 2H), ¹³C NMR (300 MHz, CDCl₃): δ 117.20, 127.42 x 2, 128.46 x 3, 128.51 x 3, 128.74 x 3, 128.94 x 3, 130.41 x 2, 132.82 x 2, 136.77 x 3, 147.1 x 3, 157.3, 159.87: ESMS: m/z 381.2 [M + 1]⁺ 333.96, 224.11

Results and discussion:

Thermochemistry

On theoretical study of the reactants 2-Phenyl-3,1-benzoxazin-4-(4H)-one (1), Indole-2carbohydrazide (2) and ethanol used as a solvent. The reaction mixture was reflux and monitoring the reaction mixture through thin layer chromatography. After completion of reaction, solvent was removed in vaccuo, to furnished the final product, N-(4-oxo-2phenylquinazolin-3(4H)-yl)-1H-indole-2-carboxamide (3) in Scheme 1 The value of Enthalpy (H/a.u.), Gibbs free energy (G/ a.u.) and Entropy [S(cal/mol/K)] of (3), (4), (5),(a) are obtained with help of Gaussian 09 program. These calculated thermodynamic parameter and

their change for Reaction, at 25° C are listed in Table 1. The positive values of enthalpy change (Δ H) and negative value of entropy shown that reaction is favourable however; positive value of Gibbs free energy (Δ G) change indicates that reaction is unfavourable. That is why the reaction is non-spontaneous. At 25° C, thermodynamic equilibrium constant (K_T) for this reaction is calculated as 0.99489. The value of Keq < 1 indicates that the reaction will require elevation of temperature and presence of catalyst.

UV-visible spectra

To gain insight into the nature of electronic transitions occurring in the experimental UV-visible spectrum of compound 3 time-dependent DFT (TD-DFT) calculations were performed gaseous phase as well as using the solvent parameters matching with chloroform. The basis set used for calculations was 6-31G (d,p) and the functionals were B3LYP and Cam-B3LYP. Also cLR (corrected linear response) calculations were performed using Cam-B3LYP/6-31G(d,p) parameters. The experimental and calculated UV–Vis spectra in region 250-400 nm are shown in Fig 5. The experimentally as well as theoretically calculated vertical excitation energies, wavelengths, oscillator strengths and orbital transition are itemized in Table 4. In present work, the theoretical calculation shows one more intense electronic transition at $\lambda_{max} = 292.86/298.13$ nm in gas/chloroform solvent with an oscillator strengths f = 4.2738/4.3050 and it has good agreement with the observed experimental data at λ_{max} = 297 nm in chloroform. It is further confirmed by the calculation of absorption maximum with the help of cLR methods which shows more intense electronic transition at $\lambda_{max} = 297.53/277.13$ nm in gas/chloroform solvent with an oscillator strengths f = 4.6806/4.6765 and it has good agreement with the above observed experimental data. The difference between experimental and theoretical results may be due to solvent effects. Due to this effect $\pi \to \pi^*$ in polar solvent shows bathochromic shift (red shift) however $n \rightarrow \pi^*$ shows hypsochromic shift (blue shift). In view of the theoretically calculated absorption spectra, the wavelength for the maximum absorption $(\pi \rightarrow \pi^*$ electronic transition), results from the highest occupied molecular orbital (H-1, 98) to the second excited unoccupied molecular orbital (L+2, 102) in the chloroform. Fig.8 of Supplementary material shows that the orbitals H, H-1 and H-6 are localized over C23-C24 of Indole ring, C14-C15 of benzene ring and C10–O11 of carbonyl group of benzaoxinone ring however orbitals L and L+2 are localized over C10-O11 of carbonyl group in benzaoxinone ring and N7-C8 bonds of benzaoxinone ring respectively. According to molecular orbital theory the nature of these electronic transitions are assigned to be $\pi(C23-C24) \rightarrow \pi^*(C10-O11), \pi(C14-C15) \rightarrow \pi^*(C10-O11), n(C10-O11) \rightarrow \pi^*(C10-O11), \pi(C10-O11), \pi(C10-O11))$ $\pi^*(C10-O11)$ and $\pi(C14-C15) \rightarrow \pi^*(N7-C8)$ respectively.

Vibrational analysis and theoretical prediction of spectra of the compounds

The vibrational analysis of N-(4-oxo-2-phenylquinazolin-3(4H)-yl)-1H-indole-2-carboxamide **3** has been found 45 atoms, belong to C_1 point group and possess 129 normal modes of vibration. The vibrational spectral assignments have been performed based on the recorded FT-IR spectra and theoretically analysis. The harmonic vibrational frequencies are calculated for the compound **3** by DFT/B3LYP level with 6-31G(d,p) basis of theory. The experimental, calculated frequencies and potential energy distribution (PED) of the target compound are summarized in **Table 5**.

N-H vibrations

The compound 5 possesses two NH vibrations first NH in indole ring and second is hydrazide NH vibrations. The asymmetric stretching of indolic NH calculated at 3528 cm⁻¹ whereas observed at 3400 cm⁻¹ and reported at 3402 cm⁻¹ in the IR absorption spectra [11] and hydrazide NH stretching vibration calculated at 3465 cm⁻¹ and observed stretching vibration merged in indolic NH due to exchangeable with deuterated chloroform.

C-H vibration

In general most of the hetero aromatic compounds has showed IR frequency at 3085 cm⁻¹due to asymmetric C-H stretching.[12] The compound (5) have observed bands at 3036 cm⁻¹ whereas as calculated bands at 3148 cm⁻¹ in FT-IR are assigned to C-H stretching vibrations As viewed by the PED, these modes involve approximately 92% contribution suggesting that they are stretching modes.

C-C vibrations

The C–C IR vibrations were found theoretically in the various ranges at 1021, 1083, 1301, 1315, 1463, 1575, 1596 and1604 cm⁻¹.as similar to the reported values at 1043,1303,1443, 1470, 1533 and 1601cm⁻¹[13] however observed value of C-C stretching vibrations are 1312 and 1571 cm⁻¹ respectively in FT-IR. Since the synthesized compound 5 was confirmed both theoretically and reported values.

C=O vibrations

The investigated compound 5 contain two carbonyl groups (C10=O11, C19=O21) due to asymmetric nature of molecule. The stretching vibration of both carbonyl carbons is observed at 1765 and 1610 cm⁻¹ whereas this is calculated at 1631 & 1620 cm⁻¹ in theoretical IR spectrum. The C=O stretching vibrations are reported at 1703 cm⁻¹[14]

¹H NMR and ¹³C NMR spectroscopy

2-Phenyl-3, 1-benzoxazin-4-(4H)-one 3 and Indole-2-carbohydrazide 4 product were obtained depending on the amount of equimolar proportion of ethanol using as a solvent and reaction conditions. The experimental and calculated ¹H, ¹³C NMR and chemical shifts (δ ppm) of N-(4-oxo-2-phenylquinazolin-3(4H)-yl)-1H-indole-2-carboxamide 3 are given in Table 2 & 3 and experimental spectrum is shown in Supplementary data Figs. 2 and 3 respectively. The chemical shifts have been calculated by using DFT (B3LYP) methods with 6-31G (d,p) basis set, employing GIAO approach. The experimental ¹H NMR spectrum of N-(4-oxo-2-phenylquinazolin-3(4H)-yl)-1H-indole-2-carboxamide 5 shows the presence of singlet at s 7.26 ppm for amide NH protons while the calculated value obtained at 9.13 ppm while other Indolic proton (NH) appears at 7.26 ppm as comparable to the calculated value at 8.65 ppm. The experimental ¹³C NMR spectrum shows two carbonyl carbon (C=O) signals one appears at 159.87 ppm, present in benzaoxinone ring others at 157.3 ppm that shows amide linkage. Instead of ¹H and ¹³C NMR chemical shifts, mass spectrum also shown in supplementary data Fig 4. we also confirm the molecular ion peaks mass spectrometer [M+1]⁺, corresponds to molecular formula C₂₃H₁₆N₄O₂.

NLO properties

The development of materials with large nonlinear optical (NLO) properties has great interest in the past few times. These materials find several device applications such as optical switches and electronics device [15-16]. These are very important in areas such as telecommunications, optical interconnections and signal processing [17-18.].The first order hyperpolarizability (β_0), electric dipole moment (μ) and polarizability (α) are calculated using B3LYP/6-31G(d,p) basis set from Gaussian 09W. The calculation of magnitude of total static dipole moment (μ_{tot}), isotropic polarizability (α_0), anisotropy of the polarizability, $\Delta \alpha$ and first hyperpolarizability(β_0) from complete equations as given below.

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

$$\alpha_0 = \frac{\alpha_{xx} + \alpha_{yy} + \alpha_{zz}}{3}$$

$$\alpha = 2^{-1/2} \left[(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 \right]^2$$

$$\beta_0 = (\beta_x^2 + \beta_y^2 + \beta_z^2)^2$$
And
$$\beta_x = \beta_{xxx} + \beta_{xyy} + \beta_{xzz}$$

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

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

The total molecular dipole moment and mean first hyperpolarizability is 2.2629 Debye and 10.2254×10^{-30} esu respectively, as shown in Tables 7. Total dipole moment of molecule is approximately two times greater than that of urea and first hyperpolarizability of compound **3** is twenty seven times greater than that of urea (μ and β of urea are 1.3732 Debye and 0.3728 $\times 10^{-30}$ esu, 6-31G (d,p) respectively [18-21]. Considering the molecule used in the comparative purposes of the NLO properties of molecular systems. Thus, the studied compound can be regarded as a good applicant for NLO material

Chemical reactivity

The chemical reactivity of molecule is described in three ways as Global and local electronic descriptors.

1.1 Global reactivity descriptors

The chemical reactivity and site selectivity of the molecular systems have been determined on the basis of Koopman's theorem [22-23]. Global reactivity descriptors as electro negativity (χ)= – $1/2(\varepsilon_{LUMO} + \varepsilon_{HOMO})$, chemical potential (μ) = 1/2 ($\varepsilon_{LUMO} + \varepsilon_{HOMO}$), global hardness (η) = 1/2 ($\varepsilon_{LUMO} - \varepsilon_{HOMO}$) $\varepsilon_{\text{HOMO}}$), global softness (S) = $1/2\eta$ and electrophilicity index (ω) = $\mu^2/2\eta$ are highly successful in predicting global reactivity trends [24-25]. According to Parr *et al.* [26], electrophilicity index (ω) is a global reactivity index similar to the chemical hardness and chemical potential. This is positive and negative definite quantity. This new reactivity index measures the stabilization in energy when the system acquires an additional electronic charge (ΔN) from the environment. The direction of the charge transfer is completely determined by the electronic chemical potential of the molecule because an electrophile is a chemical species capable of accepting electrons from the environments and its energy must decrease upon accepting electronic charge. Therefore, its electronic chemical potential must be negative. The energies of frontier molecular orbital's (ε_{HOMO} , ε_{LUMO}), energy gap (ε_{LUMO} - $\varepsilon_{\text{HOMO}}$, electronegativity (χ), chemical potential (μ), global hardness (η), global softness (S), global electrophilicity index (ω) for (1), (2), (3) and ECT for reactant system [(1) \leftrightarrow (2)] are listed in Table 10. The global electrophilicity index ($\omega = 3.357$ eV) for (3) shows that it behaves as a strong electrophile.

Electrophilic charge transfer (ECT) = $(\Delta N_{\text{max}})_{\text{A}}$ - $(\Delta N_{\text{max}})_{\text{B}}$ is defined as the difference between the ΔN_{max} = $-\mu/\eta$ values of interacting molecules. If we consider two molecules (1) and (2) approach to each other (i) if ECT > 0, charge flow from (2) to (1) (ii) if ECT < 0, charge flow from (1) to (2) [27-28]. ECT is calculated as 0.3773 *i.e* ECT > 0 for reactant system [(1) \leftrightarrow (2)], which indicates that charge flows from (2) to (1). Therefore, (1) acts as electron acceptor (electrophile) and (2) is electron donor (nucleophile). The high value of elecrophilicity index and low value of chemical potential for (1) also favours its electrophilic behaviour. In same way, the low value of electrophilicity index and high value of chemical potential for (2) also favours its nucleophilic nature.

Molecular electrostatic potential

The molecular electrostatic potential (MESP) is related to the electronic density and is a very useful descriptor for determining sites for electrophilic as well as nucleophilic attack and hydrogen-bonding interactions [29-31]. These are also provides a visual method to understand the relative polarity of a molecule and molecular electrostatic potential counter map are made by B3LYP/6-31G(d,p) method using Gauss view 9.0 program. The molecular electrostatic potential contour surface of compound 3 is shown in the Fig 6.The different values of the electrostatic potential at the surface are represented by different colours. Potential increases in the order red < yellow < green < light blue < blue [32-34]. The colour scheme for the MESP surface is red-electron rich (partially negative charge) and related to electrophilic reactivity, yellow- slightly electron rich region; green-neutral; light blue-slightly electron deficient region and blue-electron deficient(partially positive charge) and related to nucleophilic reactivity respectively [35,36]. The MEP map represents that the region of maximum negative electrostatic potential is situated around C10 & O11 with MEP value around -5.632 a.u however the most positive region is found on N9 & N12 with a value of +5.632a.u. So, it is expected that the most preferred region for electrophilic and nucleophilic attack is around C10 & O11 and N9 & N12, respectively. The MEP maps give suitable information for that region where the compound can make hydrogen-bonding interactions.

Conclusions:

For the title compound 3 we have calculated vibrational frequencies, UV-Visible, MESP surfaces, NLO properties, ${}^{1}H$ –NMR and ${}^{13}C$ -NMR chemical shifts theoretically as well as experimentally. We found that all theoretical results have good agreement with experimental data. The ${}^{1}H$ –NMR and ${}^{13}C$ -NMR calculated by GIAO method showed good accuracy with experimental signal. We also found that title compound 3 have great biological and pharmacological significance such as antimicrobial, antileishmanial etc. the title of compound **3** is also characterized by mass spectrophotometry.

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Scheme: The scheme showed synthetic pathway of N- $(4-\infty - 2 \text{ phenylquinazolin}-3(4H)-yl)-1H-indole-2-carboxamide$ **3**Where (1) & (2) indicates reactants and 3 is product and 4 is side product in the form of water.

Figure Caption:

Scheme 1 Optimized geometry of reactants (1, 2), product (3) and side product water (4)

Figure 1 Optimized geometry product (3

Figure 2 Experimental ¹H NMR spectrum of (3) in CDCl₃ solvent

Figure 3 experimental ¹³C NMR spectrum of (**3**) in CDCl₃ solvent

Figure 4 Experimental mass spectrum

Figure 5 Experimental and theoretical UV-Visible spectrum

Figure 6 Comparison between theoretical and experimental IR spectra for (3)

Figure 7 Molecular electrostatic potential (ESP) map of (3)

Figure 8 HOMO-LUMO Transitions

Table caption:

Table 1. Calculated thermodynamic parameters: Enthalpy (H / a.u.), Gibbs free energy (G / a.u.) and Entropy [S / (cal/mol–K)] of (1), (2), (3), (4) and their change for Reaction, at 25 °C.

Table 2. Calculated and experimental ¹*H* NMR chemical shifts (δ / ppm) of compound in CDCl₃-solvent at 25 °C.

Table 3. Calculated and experimental ¹³C NMR chemical shifts (δ / ppm) of compound in CDCl₃-solvent at 25 °C.

Table 4. Calculated and experimental electronic excitations for (3): E / eV, oscillatory strength (*f*), (λ_{max} / nm) at TD–DFT/B3LYP/6–31G(d,p) and Cam-B3LYP/6–31G(d,p) level.

Table 5. Experimental and theoretical [calculated at B3LYP/6–31G(d,p) level] vibrational wavenumbers of (3) and their assignments: Wavenumbers ($\overline{\nu}/\text{cm}^{-1}$), intensity (K mmol⁻¹).

Table 6. Calculated Dipole moment (μ_0), Polarizability ($|\alpha_0|$), anisotropy of Polarizability ($\Delta \alpha$), First Hyperpolarizability (β_0) and their components, using B3LYP/6–31G(d,p).

Table 7. Calculated $\varepsilon_{\text{HOMO}}$, $\varepsilon_{\text{LUMO}}$, energy band gap ($\varepsilon_{\text{L}} - \varepsilon_{\text{H}}$), chemical potential (μ), electronegativity (χ), global hardness (η), global softness (S), global electrophilicity index (ω) for (1), (2), (3) and Elecrophilicity based charge transfer (ECT) for reactant system [(1)\leftrightarrow(2)].

Table 8. Selected electrophilic reactivity descriptors $(f_k^+, s_k^+, \omega_k^+)$ for reactant (1) and nucleophilic reactivity descriptors $(f_k^-, s_k^-, \omega_k^-)$ for reactant (2), using Mulliken atomic charges.

Table 9. Selected reactivity descriptors as Fukui functions (f_k^+, f_k^-) , local softnesses (s_k^+, s_k^-) , local electrophilicity indices (ω_k^+, ω_k^-) for (3), using Mulliken atomic charges.

Table 1. Calculated thermodynamic parameters: Enthalpy (H / a.u.), Gibbs free energy (G / a.u.) and Entropy [S / (cal/mol–K)] of (1), (2), (3), (4) and their change for Reaction, at 25 °C.

	(1)	(2)	(3)	(4)		Reaction
Н	-743.941	-587.491	-1254.848	-76.394	ΔH	0.189
G	-743.994	-587.539	-1254.925	-76.416	ΔG	0.192
S	111.080	100.183	160.658	45.116	ΔS	-5.489

Table 2. Calculated and experimental	¹ H NMR	chemical	shifts	(δ /	ppm)	of
compound in CDCl ₃ -solvent at 25 °C.		\sim				

Atom	δ calcd.	δ exp.	Assignment
H30	7.9704	8.3	dd,2H, (J=7.2 Hz) benzaoxinone ring
H31	8.3078		
H32	8.1721	8.23	d, 2H, (J=7.8 Hz) benzaoxinone ring
H33	8.7778		
H34	9.1329	7.26	s ,1H amide NH
H35	8.5855		
H36	7.9118		
H37	7.7219	7.53-7.60	
H38	7.7253		m, 5H benzene ring
H39	8.301		
H40	8.6475	7.26	S ,1H Indole ring NH
H41	7.4253	7.48	S, 1H Indole five member ring
H42	7.6691	7.69	d,1H (J = 8.01 Hz) Indole six member ring
H43	7.7659	7.80	t, 2H(J =9.0 Hz) Indole six member ring
H44	7.5753		
H45	8.1186	7.69	d, 1H (J = 8.01 Hz) Indole six member ring

Atom	δ calcd.	δ exp.	Assignment
C1	122.6973		
C2	131.296	128.94-132.82	Benzaoxinone ring
C3	125.0893		
C4	145.1814	132 54 136 77	Banzaovinone bridged head
C5	119.5752	152.54-150.77	Benzaoxinone ondged nead
C6	127.1185	128.94-132.82	Benzaoxinone ring
C8	154.9916	147.1	Benzaoxinone ring between both nitrogen
C10	162.5676	159.87	C =O groups in benzaoxinone ring
C13	131.6287	130.41	benzene ring
C14	129.7846		
C15	124.4582		\sim
C16	127.853	127.2-128.74	Benzene ring
C17	122.4702		
C18	126.1606		
C19	159.6925	157.3	C =O groups amide linkage
C20	125.1501	128.46	Indole five member ring
C23	134.9564	127.42	Indola bridgad aarbon
C24	125.7714	127.42	indole bridged carbon
C25	102.2803	128.51	Indole five member ring
C26	107.9365	N	
C27	122.2289	117 2 127 4	Multiplat indale six member ring
C28	117.0865	117.2-127.4	wantpiet moore six memoer fing
C29	119.464		

Table 3. Calculated and experimental ¹³C NMR chemical shifts (δ / ppm) of compound in CDCl₃-solvent at 25 °C.

B3LYP/6-31G(d,p)	Excitations	solvent	λ_{max}	λ_{max}	E (eV)	(f)	Assignment
			Exp.	calcd.			
		gas		318.56	3.8920	0.1040	
	99→100 (H→L)	CHCl ₃	322	326.45	3.7979		$\pi \rightarrow \pi^*$
						0.1236	
		gas		308.74	4.0158	0.3606	
	98→100 (H-1→L)						$\pi {\rightarrow} \pi^*$
		CHCl ₃	284	308.22	4.0226	0.2045	
		gas		292.86	4.2738	0.1946	
	98→102 (H-1→L+2)						$\pi \rightarrow \pi^*$
		CHCl ₃	297	298.13	4.3050	0.1946	
	93→100 (H-6→L)	gas		249.72	4.9650	0.1534	
							$n \rightarrow \pi^*$
		CHCl ₃	240	252.06	4.9583	0.1347	
Cam-B3LYP/6–	99→100 (H→L)		322	284.35	4.3602	0.5603	$\pi { ightarrow} \pi^*$
31G(d,p)	98→100 (H-1→L)		284	280.82	4.4151	0.2905	$\pi {\rightarrow} \pi^*$
iop(10/74=10)	98→102 (H-1→L+2)	gas	297	297.53	4.6806	0.2383	$\pi { ightarrow} \pi^*$
scrf=pisalr	93→100 (H-6→L)		240	229.14	5.4108	0.1052	n→π*
td=noneq			/				
Cam-B3LYP/6-	99→100 (H→L)		322	284.50	4.3580	0.5667	$\pi \rightarrow \pi^*$
31G(d,p)	98→100 (H-1→L)		284	280.95	4.4130	0.2895	$\pi \rightarrow \pi^*$
iop(10/74=10)	98→102 (H-1→L+2)	CHCl ₃	297	277.13	4.6765	0.1091	$\pi { ightarrow} \pi^*$
scrf=pisalr	93→100 (H-6→L)		240	229.21	5.4092	0.2379	$n \rightarrow \pi^*$
td=noneq							
	A A						

Table-4 Calculated and experimental electronic excitations for (3): E / eV, oscillatory strength (f), (λ_{max} / nm) at TD-DFT B3LYP/6–31G(d,p) and Cam-B3LYP/6–31G(d,p) level

$\overline{\nu}$	$\overline{\nu}$	$\overline{\nu}$	Exp.	Assignment (PED) \geq 5 %
unscal.	scaled	Exp.	IR _{in}	
3246	3119	3400	0.18	v(N22H40)(98)
3241	3114		19.29	v(C3H32)(40)v(C6H33)(14)-(\deltaas-R1)(13)-v(C16C17)(12) v(C2H31)(8)
				v(C1H30)(7)
3216	3090	3036	30.97	v(C26H42)(42)-v(C29H45)(27)-v(C28H44)(22)v(C27H43)(8)
3208	3082	2926	14.06	v(C15H36)(47)-v(C17H38)(45)v(C18H39)(4)
1698	1631	1765	57.9	v(C10O11)(43)v(C19O21)(15)-v(C5C10)(9)(\deltatrigonal-R2)(5)
1687	1620	1610	441.22	v(C19O21)(39)-v(C10O11)(13)-v(C19C20)(9)-\delta(N12H34)(7)
1670	1604		74.61	v(C1C6)(16)-v(C2C3)(13) v(C3C4)(13)-v(C5C6)(10)-(δas-R1)(7)
				-δ(C1C6H33)(6)ν(C5C10)(5)-δ(C3C4H32)(5)
1661	1596		5.81	v(C14C15)(20)v(C17C18)(19)(das-R3)(9)-v(C13C14)(6)-
				δ(C14C15H35)(6) δ(C13C18H39)(5)-ν(C13C18)(5)-ν(C16C17)(5)
1640	1575	1571	24.95	v(C16C17)(19)-v(C15C16)(17)-v(C13C18)(14)v(C13C14)(12)
				-δ(C16C17H37)(10)-(δas- R3)(9)
1601	1538	1540	295.16	v(C7N8)(46)-v(C8C13)(8)-v(C4N7)(7)(\deltaas-R2)(5)
1585	1523		180.87	$v(C20C25)(29)-v(C19O21)(10)-v(C19C20)(8)-v(C23C26)(8) \delta(as-R4)(7)$
				-δ(C20C25H41)(6) -δ(C27C28H43)(5)
1557	1496		106.72	(ρ-N9N12H34)(15) δ(C14C15H36)(10) δ(C13C18H39)(9)
				δ(C17C18H38)(8)-δ(C14C15H35)(6)-δ(N12H34)(5)v(C15C16)(5)
				-v(C13C14)(5)
1549	1488	1410	132.27	(ρ-N9N12H34)(44)-δ(N12H34)(14)v(C19N12)(7)
1521	1461		117.79	δ(C1C6H33)(20)-δ(C3C4H32)(19) v(C4C5)(14)-v(C4N7)(7)
				δ(C1C2H30)(5)
)	-v(C2C3)(5)
1427	1371		23.5	v(C27C28)(12)-v(C20N22)(10)v(C24C29)(9)-v(C28C29)(7)v(C19C20)(7)
				$-v(C23C24)(6)-\delta(as-R4)(6)\delta(C28C29H44)(5)v(C23C26)(5)-v(C26C27)(5)$
1400	1345		42.25	δ(C28C29H44)(12) -δ(C20C25H41)(10) -δ(C23C26H42)(10)-
				v(C24C25)(9) 1v(C10O11)(7)-v(C26C27)(6)v(C20N22)(5)
1389	1334		65.67	v(C4C5)(15) v(C1C6)(12) v(C2C3)(11)-v(C5C6)(10)-v(C3C4)(9)-
				v(C1C2)(8) \delta(C14C15H35)(8) \delta(C13C18H39)(6)
1383	1329		17.44	v(C8N9)(15)-v(C8C13)(13)-v(N9N12)(8) δ(C13C18H39)(7)
1368	1315		12.13	v(C13C18)(18)-v(C13C14)(16)v(C16C17)(11)v(C14C15)(11)
				-v(C15C16)(10)-v(C17C18)(9)

Table 5. Experimental and theoretical [calculated at B3LYP/6–31G(d,p) level] vibrational wavenumbers of (3) and their assignments: Wavenumbers ($\overline{\nu'}$ / cm⁻¹), intensity (K mmol⁻¹).

1354	1301	1312	152.77	v(C23C24)(15)-v(C23N22)(12)-v(C24C25)(12)v(C28C29)(9)v(C26C27)(7)
1289	1238	1268	123.77	$\delta(\text{C20N22H40})(25)\delta(\text{C23C26H42})(14)\nu(\text{C23C26})(12) - 1\nu(\text{C10O11})(11)$
				$\delta(as-R4)(6)-v(C24C25)(5)$
1276	1226	1262	97.48	(δtrigonal-R5)(13)v(C23N22)(12) -1v(C10O11)(8) -δ(C20N22H40)(7)
				-v(C24C25)(7)-v(C24C29)(6)v(C19C20)(5)-v(C19N12)(5)
1272	1222	1252	134.25	ν(C10N9)(10)ν(C7N8)(10) ν(C4N7)(9)-(δtrigonal-R1)(9) δ(C1C6H33)(8)
				-v(C8N9)(6)-v(N9N12)(5)-v(C5C10)(5)
1262	1213	1207	67.88	δ(C20C25H41)(11)-v(N9N12)(11)-v(C3C4)(7)v(C19N12)(6)v(C5C10)(6)
				-δ(C20N22H40)(6)-v(C24C25)(5)-δ(C3C4H32)(5)(δtrigonal-R5)(5)
1232	1184		81.49	δ(C20C25H41)(23)v(N9N12)(11)-δ(C1C2H30)(8)δ(C28C29H44)(6)
				-v(C19C20)(6) -δ(C27C28H43)(5)
1209	1162	1078	52.01	δ(C27C28H43)(15)δ(C23C26H42)(12) -δ(C28C29H44)(11)
				1v(C10O11)(9) \delta(C20C25H41)(6) \delta(C3C4H32)(5) - \delta(C2C3H31)(5)
				-v(C24C25)(5)
1169	1123	1021	22.61	v(C10N9)(28)-v(C8N9)(14)-(8trigonal-R3)(6)
1137	1093	1012	12.28	v(C20N22)(18)-v(C19N12)(15)\delta(C20C25H41)(15)(\delta trigonal-
				R1)(5)\delta(C20N22H40)(5)
930	894	965	28.52	$(\delta trigonal-R1)(22)-(\delta trigonal-R5)(16)(\delta trigonal-R2)(9)-\delta(as-R4)(7)$
852	818	856	33.38	ω(C25H41)(42) δ00p(C19C20)(19)(τ-R4)(13) -δip(C19C20)(7)
				$-(\tau - R4)(5)(\omega - C27H43)(5)$
808	777		18.76	(ω-C1H30)(23)-(R1-Puckering)(10)(ω-C2H31)(8)(ω-C6H33)(8)
				$(R2-Puckering)(7)(\omega-C3H321)(5)$ $\delta oop(C8C13)(5)$
805	774	765	62.74	(R3-Puckering)(22) -δ00p(C8C13)(21)(ω-C16H37)(13)(ω-C1H30)(8)
777	746	734	91.68	(ω-C27H43)(20)(ω-C28H44)(19)-(ω-C26H42)(16)δip(C19C20)(16)
				(ω– C29H45)(14) -δοοp(C19C20)(10)
679	653	684	20.36	(δas-R1)(21) δ(C5C10O11)(14)-(R3-Puckering)(12)-(δas-R1)(7)
657	632	606	84.41	$\omega(N22H40)(81)(\tau - R4)(8)$

Proposed assignment and potential energy distribution (PED) for vibrational modes: Types of vibrations: ν - stretching, δ sc - scissoring, ρ - rocking, ω - wagging, δ -deformation, δ s - symmetric deformation, δ as - asymmetric deformation, τ - torsion.

	Dipole moment		Polarizability	Hyperpolarizabilit	ty
μx	0.7712	αxx	421.274	βxxx -10	78.2
μу	2.127	αуу	35.5001	βxxy 371	.327
μz	-0.0406	αzz	266.416	βхуу -19	1.64
μ	2.2629	αχγ	-42.771	βууу -34	4.42
		αxz	21.3624	βxxz 113	.962
		αyz	195.622	βxyz -64	.047
		αΟ	35.7256	βyyz 17.0	0475
		$\Delta \alpha$	119.066	βxzz 93.3	3451
				βyzz 32.2	2971
				βzzz -16	.282
		24		β0 10.2	2254

Table 6. Calculated Dipole moment (μ_0) , Polarizability $(|\alpha_0|)$, anisotropy of Polarizability $(\Delta \alpha)$, First Hyperpolarizability (β_0) and their components, using B3LYP/6–31G(d,p).

 μ_0 in Debye; $|\alpha_0|$ and $\Delta \alpha$ in 10^{-24} esu; β_0 in 10^{-30} esu,

Table 7. Calculated $\varepsilon_{\text{HOMO}}$, $\varepsilon_{\text{LUMO}}$, energy band gap ($\varepsilon_{\text{L}} - \varepsilon_{\text{H}}$), chemical potential (μ), electronegativity (χ), global hardness (η), global softness (S), global electrophilicity index (ω) for (1), (2), (3) and Elecrophilicity based charge transfer (ECT) for reactant system [(1) \leftrightarrow (2)].

	\mathcal{E}_{H}	£L	$\mathcal{E}_{L} - \mathcal{E}_{H}$	X	μ	η	S	(ω)	ЕСТ
(1)	-6.3413	-1.8825	4.4588	1119	-4.1119	2.2294	1.1147	3.7920	0.3773
(2)	-5.5832	-1.0569	4.5263	3.3200	-3.3200	2.2631	1.1315	4.5263	
(3)	-5.9710	-1.6488	4.3225	3.8097	-3.8097	2.1612	1.0806	3.3577	
8 _H , 8	l, εl-εh, χ	, μ, η, ω (i	n eV) and	S (in eV ⁻	¹) 27.2116				

Table 8. Selected electrophilic reactivity descriptors $(f_k^+, s_k^+, \omega_k^+)$ for reactant (1) and

sites	$f_{ m k}{}^+$	s_k^+	ω_k^+	sites	$f_{ m k}{}^-$	s _k ⁻	ω
C2	0.0831	0.0926	0.3151	017	0.0534	0.0604	0.2417
C3	0.0635	0.0707	0.2407	N18	0.0582	0.0658	0.2634
C6	0.0604	0.0673	0.2290	N20	0.0756	0.0855	0.3421
C8	0.0974	0.1085	0.3693				
C10	0.1115	0.1262	0.5047				
$f_{\mathrm{k}}^{+}, f_{\mathrm{k}}^{-}$	$(in e); s_k^+, s$	k^{-} (in eV ⁻¹) and	ω_k^+, ω_k^- (in e	eV)			
						X	

nucleophilic reactivity descriptors (f_k, s_k, ω_k) for reactant (2), using Mulliken atomic charges.

Table 9. Selected reactivity descriptors as Fukui functions (f_k^+, f_k^-) , local softnesses (s_k^+, s_k^-) , local electrophilicity indices (ω_k^+, ω_k^-) for (3), using Mulliken atomic charges.

sites	$f_{ m k}{}^+$	s_k^+	ω_{k}^{+}	sites	$f_{ m k}^{-}$	s _k ⁻	$\omega_{\rm k}$	
C1	0.0699	0.0755	0.2347	N7	0.0413	0.0446	0.1386	
C2	0.0599	0.0647	0.2011	N9	0.0063	0.0068	0.0211	
C16	0.0681	0.0735	0.2286	011	0.0416	0.0449	0.1396	
C25	0.0662	0.0715	0.2222	N12	0.0187	0.0202	0.0627	
C27	0.0592	0.0639	0.1987	O21	0.0237	0.0256	0.0795	
C29	0.0596	0.0644	0.2001					
$f_{ m k}{}^{_+},f_{ m k}{}^{}$	f_k^+, f_k^- (in e); s_k^+, s_k^- (in eV ⁻¹) and ω_k^+, ω_k^- (in eV)							

Figure Caption



Scheme 1 Optimized geometry of reactants (1, 2), product (3) and side product water (4)





Figure 2 Experimental ¹H NMR spectrum of (3) in CDCl₃ solvent





Figure 3 experimental ¹³C NMR spectrum of (**3**) in CDCl₃ solvent



Figure 4 Experimental mass spectrum



Figure 5 Experimental UV-Visible spectrum



Figure 6 Comparison between theoretical and experimental IR spectra for (3)



Figure 7 Molecular electrostatic potential (ESP) map of (3)



Figure 8 HOMO-LUMO Transitions

Scheme :



Scheme 1: The above scheme showed synthetic pathway of N-(4-oxo-2 phenylquinazolin-3(4H)-yl)-1H-indole-2-carboxamide **3** Where (1) & (2) indicates reactants and 3 is product and 4 is side product in the form of water.

HIGHLIGHTS

- All Experimental spectral data have good agreement with theoretical data.
- Lower value of Global electrophilicity index (ω) represents compound 3 to be a strong nucleophile.
- First hyperpolarizability (β 0) of 10.2254 × 10⁻³⁰ esu shows good NLO response.
- Various electronic transition in compound 3 predicted with the help of TD-DFT/B3LYP 6-31(d,p) and Cam-B3LYP/6-31G(d,p) set.
- MESP map is responsible for prediction of both electrophilic and nucleophilic reactive behavior.

B3LYP/6-31G(d,p) **Excitations** (*f*) solvent λ_{max} λ_{max} E (eV) Assignment Exp. calcd. 318.56 0.1040 3.8920 gas 99→100 (H→L) 322 CHCl₃ 326.45 3.7979 $\pi \rightarrow \pi^*$ 0.1236 4.0158 0.3606 gas 308.74 98→100 (H-1→L) $\pi \rightarrow \pi$ 284 4.0226 0.2045 CHCl₃ 308.22 292.86 4.2738 0.1946 gas 98→102 (H-1→L+2) $\pi \rightarrow \pi$ 297 298.13 4.3050 0.1946 CHCl₃ 4.9650 93→100 (H-6→L) 249.72 0.1534 gas $n \rightarrow \pi$ CHCl₃ 240 252.06 4.9583 0.1347 Cam-B3LYP/6-99→100 (H→L) 322 284.35 4.3602 0.5603 $\pi \rightarrow \pi^*$ 31G(d,p) 284 $98 \rightarrow 100 (H-1 \rightarrow L)$ 280.82 4.4151 0.2905 $\pi \rightarrow \pi^*$ iop(10/74=10) gas 297 $98 \rightarrow 102 (H-1 \rightarrow L+2)$ 297.53 4.6806 0.2383 $\pi \rightarrow \pi^*$ scrf=pisalr 93→100 (H-6→L) 240 5.4108 229.14 0.1052 $n {
ightarrow} \pi^*$ td=noneq Cam-B3LYP/6-99→100 (H→L) 322 284.50 4.3580 0.5667 $\pi \rightarrow \pi^*$ 31G(d,p) 98→100 (H-1→L) 284 280.95 4.4130 0.2895 $\pi{\rightarrow}\pi^*$ iop(10/74=10) $98 \rightarrow 102 (H-1 \rightarrow L+2)$ CHCl₃ 297 277.13 4.6765 0.1091 $\pi \rightarrow \pi^*$ 93→100 (H-6→L) scrf=pisalr 240 229.21 5.4092 0.2379 $n \rightarrow \pi^*$ td=noneq

Table-4 Calculated and experimental electronic excitations for (3): E / eV, oscillatory strength (f), (λ_{max} / nm) at TD-DFT B3LYP/6–31G(d,p) and Cam-B3LYP/6–31G(d,p) level

$\overline{\nu}$	$\overline{\nu}$	$\overline{\nu}$	Exp.	Assignment (PED) \geq 5 %
unscal.	scaled	Exp.	IR _{in}	
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3241	3114		19.29	v(C3H32)(40)v(C6H33)(14)-(\deltaas-R1)(13)-v(C16C17)(12) v(C2H31)(8)
				v(C1H30)(7)
3216	3090	3036	30.97	v(C26H42)(42)-v(C29H45)(27)-v(C28H44)(22)v(C27H43)(8)
3208	3082	2926	14.06	v(C15H36)(47)-v(C17H38)(45)v(C18H39)(4)
1698	1631	1765	57.9	v(C10O11)(43)v(C19O21)(15)-v(C5C10)(9)(\deltatrigonal-R2)(5)
1687	1620	1610	441.22	v(C19O21)(39)-v(C10O11)(13)-v(C19C20)(9)-\delta(N12H34)(7)
1670	1604		74.61	v(C1C6)(16)-v(C2C3)(13) v(C3C4)(13)-v(C5C6)(10)-(δas-R1)(7)
				-δ(C1C6H33)(6)v(C5C10)(5)-δ(C3C4H32)(5)
1661	1596		5.81	v(C14C15)(20)v(C17C18)(19)(das-R3)(9)-v(C13C14)(6)-
				δ(C14C15H35)(6) δ(C13C18H39)(5)-ν(C13C18)(5)-ν(C16C17)(5)
1640	1575	1571	24.95	v(C16C17)(19)-v(C15C16)(17)-v(C13C18)(14)v(C13C14)(12)
				-δ(C16C17H37)(10)-(δas- R3)(9)
1601	1538	1540	295.16	v(C7N8)(46)-v(C8C13)(8)-v(C4N7)(7)(\deltaas-R2)(5)
1585	1523		180.87	$v(C20C25)(29)-v(C19O21)(10)-v(C19C20)(8)-v(C23C26)(8) \delta(as-R4)(7)$
				-δ(C20C25H41)(6) -δ(C27C28H43)(5)
1557	1496		106.72	(ρ- N9N12H34)(15) δ(C14C15H36)(10) δ(C13C18H39)(9)
				δ(C17C18H38)(8)-δ(C14C15H35)(6)-δ(N12H34)(5)v(C15C16)(5)
				-v(C13C14)(5)
1549	1488	1410	132.27	(ρ-N9N12H34)(44)-δ(N12H34)(14)ν(C19N12)(7)
1521	1461		117.79	δ(C1C6H33)(20)-δ(C3C4H32)(19) ν(C4C5)(14)-ν(C4N7)(7)
				δ(C1C2H30)(5)
				-v(C2C3)(5)
1427	1371		23.5	v(C27C28)(12)-v(C20N22)(10)v(C24C29)(9)-v(C28C29)(7)v(C19C20)(7)
				$-v(C23C24)(6)-\delta(as-R4)(6)\delta(C28C29H44)(5)v(C23C26)(5)-v(C26C27)(5)$
1400	1345		42.25	δ(C28C29H44)(12) -δ(C20C25H41)(10) -δ(C23C26H42)(10)-
				v(C24C25)(9) 1v(C10O11)(7)-v(C26C27)(6)v(C20N22)(5)
1389	1334		65.67	v(C4C5)(15) v(C1C6)(12) v(C2C3)(11)-v(C5C6)(10)-v(C3C4)(9)-
				v(C1C2)(8) \delta(C14C15H35)(8) \delta(C13C18H39)(6)
1383	1329		17.44	v(C8N9)(15)-v(C8C13)(13)-v(N9N12)(8) δ(C13C18H39)(7)
1368	1315		12.13	v(C13C18)(18)-v(C13C14)(16)v(C16C17)(11)v(C14C15)(11)
				-v(C15C16)(10)-v(C17C18)(9)

Table 5. Experimental and theoretical [calculated at B3LYP/6–31G(d,p) level] vibrational wavenumbers of (3) and their assignments: Wavenumbers ($\overline{\nu'}$ / cm⁻¹), intensity (K mmol⁻¹).

1354	1301	1312	152.77	v(C23C24)(15)-v(C23N22)(12)-v(C24C25)(12)v(C28C29)(9)v(C26C27)(7)
1289	1238	1268	123.77	$\delta(\text{C20N22H40})(25)\delta(\text{C23C26H42})(14)\nu(\text{C23C26})(12) - 1\nu(\text{C10O11})(11)$
				$\delta(as-R4)(6)-v(C24C25)(5)$
1276	1226	1262	97.48	$(\delta trigonal-R5)(13)v(C23N22)(12) -1v(C10O11)(8) -\delta(C20N22H40)(7)$
				-v(C24C25)(7)-v(C24C29)(6)v(C19C20)(5)-v(C19N12)(5)
1272	1222	1252	134.25	ν(C10N9)(10)ν(C7N8)(10) ν(C4N7)(9)-(δtrigonal-R1)(9) δ(C1C6H33)(8)
				-v(C8N9)(6)-v(N9N12)(5)-v(C5C10)(5)
1262	1213	1207	67.88	δ(C20C25H41)(11)-v(N9N12)(11)-v(C3C4)(7)v(C19N12)(6)v(C5C10)(6)
				-δ(C20N22H40)(6)-v(C24C25)(5)-δ(C3C4H32)(5)(δtrigonal-R5)(5)
1232	1184		81.49	δ(C20C25H41)(23)v(N9N12)(11)-δ(C1C2H30)(8)δ(C28C29H44)(6)
				-v(C19C20)(6) -δ(C27C28H43)(5)
1209	1162	1078	52.01	δ(C27C28H43)(15)δ(C23C26H42)(12) -δ(C28C29H44)(11)
				1v(C10O11)(9) \delta(C20C25H41)(6) \delta(C3C4H32)(5) - \delta(C2C3H31)(5)
				-v(C24C25)(5)
1169	1123	1021	22.61	v(C10N9)(28)-v(C8N9)(14)-(8trigonal-R3)(6)
1137	1093	1012	12.28	v(C20N22)(18)-v(C19N12)(15)\delta(C20C25H41)(15)(\deltatrigonal-
				R1)(5)\delta(C20N22H40)(5)
930	894	965	28.52	(δtrigonal-R1)(22)-(δtrigonal-R5)(16)(δtrigonal-R2)(9)-δ(as-R4)(7)
852	818	856	33.38	ω(C25H41)(42) δ00p(C19C20)(19)(τ-R4)(13) -δip(C19C20)(7)
				$-(\tau - R4)(5)(\omega - C27H43)(5)$
808	777		18.76	(ω-C1H30)(23)-(R1-Puckering)(10)(ω-C2H31)(8)(ω-C6H33)(8)
				$(R2-Puckering)(7)(\omega-C3H321)(5)$ $\delta oop(C8C13)(5)$
805	774	765	62.74	(R3-Puckering)(22) -δοοp(C8C13)(21)(ω–C16H37)(13)(ω–C1H30)(8)
777	746	734	91.68	(@-C27H43)(20)(@-C28H44)(19)-(@-C26H42)(16)δip(C19C20)(16)
				(ω– C29H45)(14) -δοοp(C19C20)(10)
679	653	684	20.36	(δas-R1)(21) δ(C5C10O11)(14)-(R3-Puckering)(12)-(δas-R1)(7)
657	632	606	84.41	ω(N22H40)(81)(τ-R4)(8)

Proposed assignment and potential energy distribution (PED) for vibrational modes: Types of vibrations: ν stretching, δ sc – scissoring, ρ – rocking, ω – wagging, δ -deformation, δ s – symmetric deformation, δ as – asymmetric deformation, τ – torsion.

xx0.7712αxx421.274βxxx-1078.3xy2.127αyy35.5001βxxy371.323zz-0.0406αzz266.416βxyy-191.64a2.2629αxy-42.771βyyy-344.43αxz21.3624βxxz113.962αyz195.622βxyz-64.047α035.7256βyyz17.0475Δα119.066βxzz93.3453ββyzz32.2973βββ10.2254μββ10.2254	Dipol	e moment	Polarizability		Hyperp	olarizability
μy2.127 $\alpha y y$ 35.5001 $\beta x x y$ 371.327 $1z$ -0.0406 $\alpha z z$ 266.416 $\beta x y y$ -191.64 $1z$ 2.2629 $\alpha x y$ -42.771 $\beta y y y$ -344.42 $\alpha x z$ 21.3624 $\beta x x z$ 113.962 $\alpha y z$ 195.622 $\beta x y z$ -64.047 $\alpha 0$ 35.7256 $\beta y y z$ 17.0475 $\alpha 0$ 35.7256 $\beta y y z$ 17.0475 $\alpha 0$ 35.7256 $\beta y y z$ 32.2975 $\alpha 0$ $\beta z z z$ -16.282 $\alpha 0$ $\beta 0$ 10.2254 $\alpha 0$ $\alpha n 10^{-24} esu; \beta_0 in 10^{-30} esu,$	ιx	0.7712	αχχ	421.274	βxxx	-1078.2
$1z$ -0.0406 αzz 266.416 βxyy -191.64 2.2629 αxy -42.771 βyyy -344.42 αxz 21.3624 βxxz 113.962 αyz 195.622 βxyz -64.042 $\alpha 0$ 35.7256 βyyz 17.0475 $\alpha 0$ 35.7256 βyyz 17.0475 $\alpha 0$ 119.066 βxzz 93.3452 $\alpha 0$ βyzz 32.2972 $\alpha 0$ βyzz 32.2972 $\alpha 0$ βxzz 93.3452 $\beta 0$ 10.2254 $\beta 0$ 10.2254	ly	2.127	αγγ	35.5001	βхху	371.327
2.2629 αxy -42.771 βγγγ -344.42 αxz 21.3624 βxxz 113.962 αyz 195.622 βxyz -64.042 $\alpha 0$ 35.7256 βyyz 17.0475 $\alpha 0$ 35.7256 βyyz 93.3452 $\alpha 0$ 119.066 βxzz 93.3452 $\alpha 0$ 119.066 βxzz 93.3452 $\alpha 0$ 10.2254 $\beta 0$ 10.2254 $\alpha 0$ $\alpha 0$ 10^{-24} $\alpha 0$	lZ	-0.0406	αzz	266.416	βxyy	-191.64
αxz 21.3624 βxxz 113.962 αyz 195.622 βxyz -64.042 $\alpha 0$ 35.7256 βyyz 17.0475 $\Delta \alpha$ 119.066 βxzz 93.3452 $\Delta \alpha$ 119.066 βxzz 93.3452 $\Delta \alpha$ 119.066 βxzz 93.3452 βyzz 32.2972 32.2972 βyzz 32.2972 βzzz $\beta 0$ 10.2254 μ_0 in Debye; $ \alpha_0 $ and $\Delta \alpha$ in 10 ⁻²⁴ esu; β_0 in 10 ⁻³⁰ esu,	ι	2.2629	αχγ	-42.771	βγγγ	-344.42
$\begin{array}{c c c c c c c c c c c c c c c c c c c $			αxz	21.3624	βxxz	113.962
$\alpha 0$ 35.7256 βyyz 17.0475 $\Delta \alpha$ 119.066 βxzz 93.3455 βyzz 32.2975 32.2975 βzzz -16.282 $\beta 0$ 10.2254 μ_0 in Debye; $ \alpha_0 $ and $\Delta \alpha$ in 10 ⁻²⁴ esu; β_0 in 10 ⁻³⁰ esu,			αyz	195.622	βxyz	-64.047
Δα 119.066 β_{XZZ} 93.345: β_{YZZ} 32.297: β_{ZZZ} -16.282 β_{0} 10.2254 μ_{0} in Debye; $ \alpha_{0} $ and $\Delta \alpha$ in 10 ⁻²⁴ esu; β_{0} in 10 ⁻³⁰ esu,			α0	35.7256	βyyz	17.0475
βyzz 32.297: βzzz -16.282 β0 10.2254 μ0 in Debye; $ \alpha_0 $ and $\Delta \alpha$ in 10 ⁻²⁴ esu; β_0 in 10 ⁻³⁰ esu,			Δα	119.066	βxzz	93.3451
$\beta zzz -16.28z$ $\beta 0 10.2254$ $\mu_0 \text{ in Debye; } \alpha_0 \text{ and } \Delta \alpha \text{ in } 10^{-24} \text{ esu; } \beta_0 \text{ in } 10^{-30} \text{ esu,}$					βyzz	32.2971
ι_0 in Debye; $ \alpha_0 $ and $\Delta \alpha$ in 10 ⁻²⁴ esu; β_0 in 10 ⁻³⁰ esu,				~	βzzz	-16.282
ι_0 in Debye; $ \alpha_0 $ and $\Delta \alpha$ in 10^{-24} esu; β_0 in 10^{-30} esu,					β0	10.2254
	U	5 71 01			,	

Figure



Figure 1 Optimized geometry product (3)



Figure 2 Experimental ¹H NMR spectrum of (3) in CDCl₃ solvent



Figure 5 Experimental UV-Visible spectrum



Figure 6 Comparison between theoretical and experimental IR spectra for (3)



Figure 7 Molecular electrostatic potential (ESP) map of (3)