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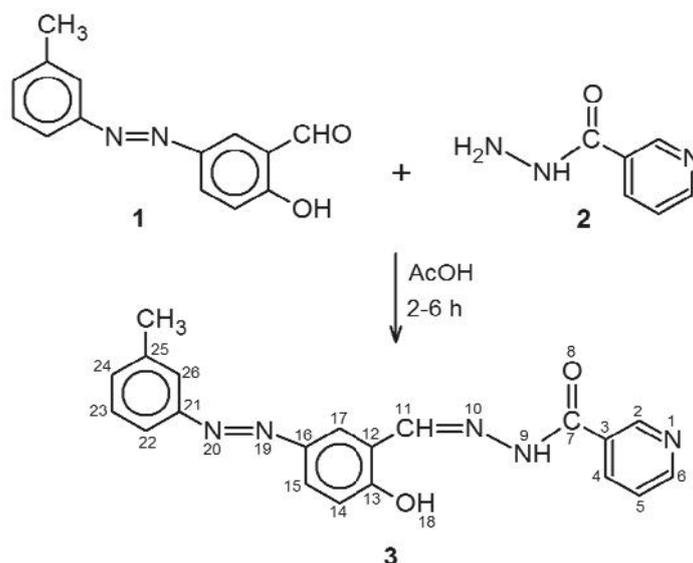## SYNTHESIS AND SPECTRAL STUDIES ON Nʹ-(5-M-METHYLPHENY LAZOSALICYLIDEN) NICOTINOHYDRAZIDE: A DFT APPROACH

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RESEARCH ARTICLE

SYNTHESIS AND SPECTRAL STUDIES ON N′-(5-M-METHYLPHENY LAZOSALICYLIDENE)NICOTINOHYDRAZIDE: A DFT APPROACH

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ABSTRACT

N'-(5-m-Methylphenylazosalicyliden)nicotinohydrazide **3** is synthesized from the condensation of N'-5-m-methylphenylazosalicylaldehyde **1** with nicotinohydrazide **2**. 5-m-Methylphenylazosalicylaldehyde was prepared by diazotization of m-methylaniline and then the coupling reaction with salicylaldehyde. This compound was characterized by IR, ^{1}H and ^{13}C NMR spectral studies. The structure of the compound are optimized and studied by B3LYP density functional method calculations at 6-31G(d,p) basis set using Gaussian-03 software. Stability of the compound has been analyzed by calculating the intramolecular charge transfer (ICT) using natural bond orbital (NBO) analysis. Topological properties of the electronic charge density were analyzed employing the Bader's atoms in molecular (AIM) theory, which indicated the presence of intramolecular hydrogen bond in the molecules. The first order hyperpolarizaibility (The first order hyperpolarizaibility (tot) and polarizability (0) were calculated using 6-31G(d,p) basis set and the nonlinear optical (NLO) properties are also addressed theoretically.

INTRODUCTION

Hydrazide derivatives have been of great interest because of their role in natural and synthetic organic chemistry. Many products, which contain a hydrazide subunit exhibit biological activity such as molluscicides, anthelmintic, hyponotic, insecticidal activity (Williams and Lemke, 2002) and fluorescent brightness. Many hydrazone compounds showed good anticancer bioactivities (Prescott *et al.,* 1990). Hydrazone functional group increases the lipophilicity of parent amine and amides and results in the enhancement of absorption through biomembranes and enables them to cross bacterial and fungal membranes (Madhukar *et al.,* 2009; Jha *et al.,* 2010). The pyridyl ring, a prominent scaffold present in plenty of bioactive molecules has played a vital role in the development of different medicinal agents. Hydrazides have recently become attractive to theoreticians as well as experimentalists due to the biological significance particularly in medicinal and enzyme chemistry. Schiff base hydrazones are widely used in analytical chemistry as selective metal extracting agents as well as in spectroscopic determination of certain transition metal (Gallego *et al.,* 1979; Gallego *et al.,* 1978).

Conformational analysis of hydrazones from spectral studies were also reported in literature (Bessy Raj and Prathapachandra Kurup, 2007; Benassi *et al.,* 2005; Manimekalai *et al.,* 2004;

Hosny, 2009). Organic molecules with conjugated π-electron system are known to exhibit extremely large optical nonlinear responses in terms of their molecular hyperpolarizability values, which depend not only on the strength of donor and acceptor groups but also on the path length between them (Prasad and Williams, 1991; Karakas *et al.,* 2005). Recently, second order NLO effects of organic molecules have been extensively investigated for their advantages over inorganic crystals and they play an important role in second harmonic generation, frequency mixing and electro-optic modulation (Badan *et al.,* 1993).

Experimental

Nicotinohydrazides was purchased from sigma Aldrich. All other chemicals were used as analytic grade. Reaction was monitored by TLC. The melting point is measured on open capillaries and are in corrected.

Synthesis of N′-(5-m-Methylphenylazosalicylidene) nicotinohydrazide 3

N'-(5-m-Methylphenylazosalicyliden)nicotinohydrazide **3** was prepared according to the procedure reported by Odabasoglu *et al.* (2007). To solution of N'-5-m methylphenylazosalicylaldehyde **1** (0.01 mol, 1.371 g) and

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nicotinohydrazide **2** (0.01 mol, 2.3 g) in methanol five drops of glacial acetic acid were added and the reaction mixture was refluxed for 6 h and then the mixture was poured into ice cold water. The mixture was kept over night at room temperature. It was filtered, washed and recrystallized from methanol. Yield was found to be 83%, colour: orange; m.p. 197–199°C.

Spectral Measurements

The FT-IR spectrum is recorded in the range 4000–400 cm^{-1} with a resolution of ±4 cm^{-1} and an accuracy of ±0.01 cm^{-1} on Nicolet Avatar 360 FT-IR spectrometer. The sample was mixed with KBr and the pellet technique was adopted. The proton spectrum at 400 MHz and proton decoupled ^{13}C NMR spectrum at 100 MHz in DMSO-d_6 were recorded at room temperature on Bruker 400 MHz spectrometer using 10 mm sample tube, samples were prepared by dissolving about 10 mg of the sample in 0.5 mL of DMSO-d_6 containing a few drops at TMS for ^{13}C.

Computational Studies

Geometry optimization was carried out according to density functional theory available in Gaussian-03 package using B3LYP/6-31G(d,p) basis set (Frisch *et al.,* 2001). The polarizabilities and hyperpolarizabilities were determined from the DFT optimized structures by finite field approach using B3LYP/6-31G* basis set available in Gaussian-03 package and NBO calculations using the basis set B3LYP/6-311G(d,p) (Weinhold and Landis, 2005). AIM parameters were determined using AIM All package (Keith, 2011) from B3LYP/6-31G(d,p) optimized structure.

RESULTS AND DISCUSSION

The *N′*-(5-*m*-Methylphenylazosalicyliden)nicotinohydrazide **3** is obtained by refluxing 5-*m*-methylphenylazosalicylaldehyde **1** with nicotinohydrazide **2** and 5 drops of acetic acid in methanol (Scheme 1). All the synthesized compounds are characterized by the FT-IR and the high-resolution ^{1}H and ^{13}C NMR spectra and analyzed. The theoretical vibrational frequencies of the hydrazide **3** is calculated using DFT method with 6-31G(d,p) basis set and scaled by a factor 0.9614.
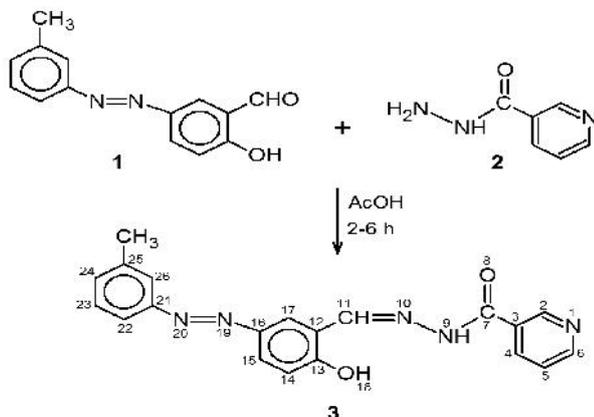
Scheme 1 Synthetic route of *N′*-(5-*m*-methylphenylazosalicyliden) nicotinohydrazide **3**

The prominent peaks in the range 3430–3190, 1650–1800 and 1640–1560 cm^{-1} in the IR spectrum are attributed to ν_{N-H} and ν_{O-H}, $\nu_{C=O}$ and $\nu_{C=N}$ and $\nu_{C=C}$ modes respectively. The observation of lower $\nu_{C=O}$ is due to the extended conjugation of C=O group with the nearby pyridine ring. The bending vibration of the O–H group appeared around 1350 cm^{-1} in all the hydrazides. The sharp peak around 3020 cm^{-1} in the IR spectrum of **3** due to the aromatic ν_{C-H} mode. In hydrazide strong peak for N=N group is observed at 1480 cm^{-1}. Aromatic C–H out-of-plane bending vibration appeared around 840 and 700 cm^{-1}. The experimental and calculated (DFT) IR spectral data of **3** is displayed in Table 1 and the IR spectrum of hydrazide **3** is shown in Fig. 1.

Spectral (^{1}H and ^{13}C NMR) Calculation

The signals in the ^{1}H NMR spectrum (Fig. 2) were assigned based on their positions, integrals, multiplicities and on comparison with those signals of 5-phenylazosalicylaldehyde. In ^{13}C NMR spectrum (Fig. 3) quaternary carbons can be easily distinguished from other carbons based on small intensities. The ^{1}H and ^{13}C NMR chemical shifts were determined theoretically by DFT method in DMSO-d_6 using the basis set B3LYP/6-311+G(2d,p) GIAO and the salvation model PCM (SCRF=PCM) (Miertus and Tomasi, 1982).
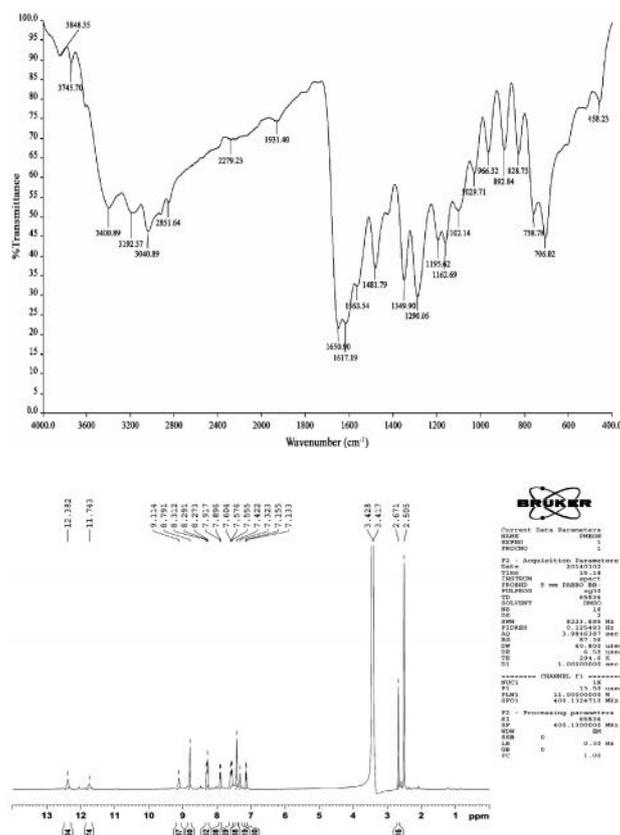
Fig. 2 ^{1}H NMR spectrum of *N′*-(5-*m*-methylphenylazosalicyliden)nicotinohydrazide **3**

The ^{1}H and ^{13}C chemical shifts relative to reference material TMS are determined from the shielding tensors using the scale factors 31.8821 and 182.4656 respectively and they are listed in Table 2 itself. The scale factors are based on the reference

compounds used as well as on the basis set employed for DFT calculation. Theoretically determined ^{1}H chemical shifts are generally high when compared to experimental values and large derivatives are noted on some protons. The experimental ^{13}C chemical shifts are however closer to the theoretical values. Experimental and computational ^{1}H and ^{13}C NMR spectral data of hydrazide **3** are listed in Table 2.

Fig. 3 ^{13}C NMR spectrum of *N′*-(5-*m*-methylphenylazosalicyliden)nicotinohydrazide **3**

Table 1 Experimental and computational IR spectral data (cm^{−1}) of *N′*-(5-*m*-methylphenylazosalicyliden)nicotinohydrazide **3**

Observed	DFT
3401	3404
3193	3249
3041	3030
1651	1626
1617	1601
1564	1564
1482	1503
1350	1332
1290	1285
1196	1229
1163	1150
1102	1092
1030	1060
966	964
893	882
829	834
759	755
706	697
458	461

AIM Analysis

Atoms in molecules electron density topological analysis carried out for hydrazide **3** using AIM All package (Keith, 2011) revealed the existence of 44 bond critical point (BCP) with (3, −1) topology. Table 3 lists ρ_{BCP}, $\nabla^2\rho_{BCP}$, ε, the three eigen values λ_1, λ_2 and λ_3, the relationship between the perpendicular and parallel curvatures $|\lambda_1|/\lambda_3$, the potential energy density V, the kinetic energy density G, the total energy density H and the kinetic energy density for charge unit G/ρ_{BCP} values for some selected bonds and ρ values of ring critical points (RCP) of hydrazide **3**.

For shared (covalent) interaction between two atoms charge density at BCP is very high ($\rho_{BCP} \approx 10^{−1}$ a.u), whereas for closed shell interactions ρ_{BCP} is small ($\approx 10^{−3}$ a.u). The high values of ρ_{BCP} (Table 3) observed for all bonds except between non-bonded atoms N10···H18 indicate the interaction between two atoms is covalent in nature. In addition to charge density,

Table 2 Experimental and computational ^{1}H and ^{13}C NMR spectral data (ppm) of *N′*-(5-*m*-methylphenylazosalicyliden)nicotinohydrazide **3**

Protons	Observed	DFT
H–2	9.11	9.33
H–4	8.30	8.82
H–5	7.57	7.87
H–6	8.79	9.15
H–11	8.79	8.58
H–14	7.14	7.55
H–15	7.91	8.48
H–17	8.27	8.52
H–22	7.60	8.34
H–23	–	–
H–24	7.32	7.81
H–25	7.42	7.96
H–26	7.42	8.23
CH$_3$	2.41	2.55
Carbons		
C–2	148.47	153.66
C–3	130.78	135.13
C–4	135.56	144.03
C–5	123.76	129.56
C–6	152.44	160.71
C–7	161.69	167.54
C–11	147.16	153.92
C–12	119.41	124.36
C–13	159.97	171.23
C–14	117.34	121.63
C–15	125.10	143.68
C–16	145.57	152.15
C–17	124.43	121.75
C–21	149.91	159.55
C–22	115.07	117.68
C–23	137.01	147.79
C–24	126.56	139.36
C–25	131.32	134.35
C–26	131.32	135.72
CH$_3$	17.05	22.25

Laplacian of the charge density also provides information about covalent and closed shell interactions present in the molecule. The negative values obtained for the Laplacian of electron density ($\nabla^2\rho_{BCP}$) for N1–C2, N1–C6, C3–C7, C7–O8, C7–N9, N9–N10, N10–C11, C13–O18, C16–N19, N19–N20, C21–N20, N9–H9 and O18–H18 are a clear indication that the electronic charge is locally arranged within the region of inter atoms leading to an interaction named as covalent or polarized bonds and being characterized by large ρ values (Lesar and Milosev, 2009; Huyskens *et al.,* 1998).

Besides these BCP was located between the non-bonded H(18) and N(10) atoms in hydrazide **3**. The ρ_{BCP} values obtained in the present study and positive magnitude of $\nabla^2\rho_{BCP}$ reported in Table 3 are in the high limit of the requirements to define a hydrogen bond and thus a strong interaction may be inferred.

Ring critical point of phenyl ring attached to N(20) is slightly having higher electron density compared to the phenolic ring. Another ring critical point was also observed in hydrazide [C(12)–C(13)–O(18)–H(18)–N(10)–C(11)] thus reinforcing the idea of a strong intramolecular hydrogen bond for the hydrazide **3**. As pointed by Bader (Sun and Hu, 2005; Amoozadeh *et al.,* 2013) a relationship exists between the hydrogen bond strength and the density in the BCP.

Table 3 Topological properties at BCP (3, –1) in relevant bonds and RCPs of
N′-(5-*m*-methylphenylazosalicyliden)nicotinohydrazide **3**

Bond (A···B)	ρ_{BCP}	$-\nabla^2\rho_{BCP}$	v	λ_1	λ_2	λ_3	$\lvert\lambda_1\rvert/\lambda_3$	G	V	H	G/ρ_{BCP}
N1–C2	0.3465	1.0773	0.1277	–0.7563	–0.6707	0.3497	2.1627	0.2955	–0.8603	–0.5648	0.8528
N1–C6	0.3443	1.0428	0.1078	–0.7470	–0.6743	0.3785	1.9736	0.3033	–0.8673	–0.5640	0.8809
C3–C7	0.2657	0.6613	0.1009	–0.5417	–0.4920	0.3724	1.4546	0.0614	–0.2881	–0.2267	0.2311
C7–O8	0.4075	0.0657	0.1037	–1.0636	–0.9637	2.0930	0.5082	0.7150	–1.4136	–0.6986	1.7546
C7–N9	0.3069	0.9350	0.1174	–0.6693	–0.5990	0.3334	2.0075	0.2319	–0.6976	–0.4657	0.7556
N9–N10	0.3584	0.7059	0.0885	–0.8126	–0.7465	0.8532	0.9524	0.1784	–0.5332	–0.3549	0.4978
N10–C11	0.3674	0.5358	0.2674	–0.8559	–0.6753	0.9954	0.8599	0.4960	–1.1260	–0.6300	1.3500
C13–O18	0.3075	0.3483	0.0083	–0.6612	–0.6557	0.9686	0.6826	0.3976	–0.8823	–0.4847	1.2930
C16–N19	0.3040	0.9800	0.0910	–0.6559	–0.6011	0.2770	2.3679	0.1517	–0.5484	–0.3967	0.4990
N19–N20	0.4536	1.0405	0.1327	–1.0838	–0.9569	1.0002	1.0836	0.2732	–0.8065	–0.5333	0.6023
N20–C21	0.301	0.9651	0.0672	–0.6449	–0.6043	0.2841	2.2700	0.1444	–0.5300	–0.3856	0.4797
N9–H9	0.3418	1.8103	0.0581	–1.3175	–1.2452	0.7524	1.7511	0.0538	–0.5603	–0.5064	0.1574
O18–H18	0.3361	1.9608	0.0166	–1.7757	–1.7467	1.5615	1.1372	0.0715	–0.6333	–0.5617	0.2127
N10···H18	0.0429	–0.1123	0.0328	–0.0668	–0.0647	0.2438	0.2740	0.0301	–0.0322	–0.0020	0.7016

	Ring		**Ring parameters ($\rho \times 10^2$)**
1	N1–C6–C5–C4–C3–C2		2.2280
2	C21–C22–C23–C24–C25–C26		2.0062
3	C12–C13–C14–C15–C16–C17		1.9565
4	C12–C13–O18–H18–N10–C11		1.5965

NBO Analysis

NBO analysis of hydrazide **3** is carried out at B3LYP/6-311G(d,p) level (Weinhold and Landis, 2005) and the significant donor-acceptor interactions are exposed in Table 4. The interaction between filled and empty NBO's can be described as a hyperconjugative electron transfer process from the donor (filled) to the acceptor (vacant) orbital and the energy lowering due to this interaction is expressed as E_2. The delocalization energy corresponding to the transfer of electrons from the bonding orbital of N19–N20 to the antibonding orbital of C26–C21 (≈ 10.7 kCal mol^{-1}) is lower than that of the energy corresponding to the transfer of electrons from the bonding orbital of C26–C21 to the antibonding orbital of N19–N20 (≈ 20 kCal mol^{-1}) in hydrazide **3**. In hydrazide **3**, the delocalization energy is higher for the transfer of electrons from bonding orbital of C16–C15 to the antibonding orbital of N19–N20 (21.7 kCal mol^{-1}) compared to the reverse transfer (10.1 kCal mol^{-1}). This confirms that electron transfer occurs from phenolic ring to the azo nitrogen in hydrazide **3**.

Hydrazide **3** shows some exceptional delocalization behaviour. Charge transfer occurs from molecular unit 1 [C$_{19}$H$_{14}$N$_5$O$_2$)], to molecular unit 2 [H(18)]. Molecular unit 1 is nothing but molecular formula without phenolic hydrogen. The σ bonding electrons present in C(13)–O(18) bond are transferred to the antibonding pure *s*-orbital of H(18) [σ*H(18)]. In addition the lone pair of electrons present on oxygen atom O(18) is transferred to σ* H(18) orbital. In hydrazide **3** the strong interaction involves charge transfer from molecular unit 1 to unit 2 *i.e.,* N(10) lone pair as donor and the antibonding pure *s*-orbital of H(18) [σ*H(18)] as acceptor (32.24 kCal mol^{-1}). The delocalization energy corresponding to the hydrogen bonding is found to be around 23 kCal mol^{-1}.

NLO Properties

The polarizabilites were calculated and the values are listed in Table 5. The molecule is a polar one having non-zero dipole moment. The β_{tot} obtained by numerical second derivative of electric dipole moments according to FF approach is found to be 15.5980×10^{-30} esu.

Table 4 NBO analysis of *N′*-(5-*m*-methylphenylazosalicyliden)nicotinohydrazide **3** by DFT method [B3LYP/6-311G(d,p)]

Donor NBO	Acceptor NBO	E_2 (kCal mol^{-1})
BD(2)C3–C2	BD*(2)C7–O8	17.74
BD(2)C3–C2	BD*(2)C4–C5	20.96
BD(2)C3–C2	BD*(2)N1–C6	16.45
BD(2)C4–C5	BD*(2)C3–C2	17.83
BD(2)C4–C5	BD*(2)N1–C6	29.30
BD(2)N1–C6	BD*(2)C3–C2	27.27
BD(2)N1–C6	BD*(2)C4–C5	12.74
BD(2)C26–C21	BD*(2)N19–N20	20.24
BD(2)C26–C21	BD*(2)C22–C23	18.06
BD(2)C26–C21	BD*(2)C25–C24	19.57
BD(2)C22–C23	BD*(2)C26–C21	20.56
BD(2)C22–C23	BD*(2)C25–C24	19.68
BD(2)C25–C24	BD*(2)C26–C21	19.94
BD(2)C25–C24	BD*(2)C22–C23	19.07
BD(2)N19–N20	BD*(2)C26–C21	10.72
LP(1)N9	BD*(2)C11–N10	27.59
LP(1)N9	BD*(2)C7–O8	47.55
LP(2)O8	BD*(1)N9–C7	29.15
LP(2)O8	BD*(1)C7–C3	19.84
LP(1)N1	BD*(1)C3–C4	10.45
LP(2)O18	BD*(2)C13–C14	37.92
BD(2)C12–C17	BD*(2)C13–C14	21.54
BD(2)C12–C17	BD*(2)C16–C15	15.48
BD(2)C12–C17	BD*(2)C11–N10	25.47
BD(2)C13–C14	BD*(2)C16–C15	26.95
BD(2)C13–C14	BD*(2)C12–C17	15.50
BD(2)C16–C15	BD*(2)C12–C17	25.25
BD(2)C16–C15	BD*(2)C13–C14	17.00
BD(2)C16–C15	BD*(2)N19–N20	21.67
BD(2)N19–N20	BD*(2)C16–C15	10.11
From Unit 1 to Unit 2		
BD(1)C13–O18	LP*(1)H18	16.13
LP(1)N10	LP*(1)H18	32.24
LP(1)O18	LP*(1)H18	12.94
LP(3)O18	LP*(1)H18	440.42

This value is found to be nearly 42 times greater than that of urea 0.3728×10^{-30} esu. The microscope molecules with larger hyperpolarizability values will make macroscopic materials

with strong non-linear optical properties. The observed value indicates that the molecule **3** can be considered as a better NLO material than urea molecule.

Table 5 Polarizabilities and hyperpolarizabilities of *N′*-(5-*m*-methylphenylazosalicyliden)nicotinohydrazide **3**

Polarizability		Hyperpolarizability	
α_{xx}	573.277	β_{xxx}	−53.885
α_{xy}	31.077	β_{xxy}	−1778.552
α_{yy}	293.727	β_{xyy}	−309.157
α_{xz}	9.488	β_{yyy}	24.732
α_{yz}	6.003	β_{xxz}	168.139
α_{zz}	96.473	β_{xyz}	3.156
$<\alpha>$ (a.u)	321.159	β_{yyz}	5.619
$10^{24} \times \alpha_{tot}$ (esu)	47.596	β_{xzz}	−26.162
		β_{yzz}	−0.324
		β_{zzz}	2.951
		β_{tot} (a.u)	1805.471
		$10^{33} \times \beta_{tot}$ (esu)	15598.005

CONCLUSIONS

The hydrazide **3** is synthesized and characterized by spectral studies. The polarizability and first order hyperpolarizability were also computed and calculated. Theoretical FT-IR spectral frequencies are in good agreement with experimental data. NBO analysis shows that the transfer of electrons occurs from phenyl ring to azo linkage. The AIM analysis shows the presence of weak hydrogen bond between N10 and H18.

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