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Synthesis, molecular structure, FT-IR, FT-Raman and XRD spectroscopic investigations of (E)-1-(5-((4-bromophenyl)diazenyl)-2-hydroxyphenyl)ethanone: A comparative DFT study

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ABSTRACT

The (E)-2-acethyl-4-(4-bromophenyldiazenyl) phenol compound was synthesized and analysed by elemental analysis, single-crystal X-ray diffraction (XRD), FT-IR and FT-Raman spectroscopies. Furthermore, vibrational spectra of this compound have been assigned by using scaled quantum mechanical force field approximation from density functional method (B3LYP) with 6-31G(d) basis set. A well-agreement has been attained between the calculated and observed spectra. Moreover, NBO analysis indicates there are strong conjugate interactions inside the molecule. Apart from this, the single-crystal structure from X-ray study has showed that this compound has a strong intramolecular O—H … O hydrogen bond and $\pi - \pi$ stacking.

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1. Introduction

Azobenzenes are chemical compounds considered as derivatives of organic diazenes. As containing π-congugation in the structure, they absorb light efficiently. Therefore, they have been mainly used as dyes and pigments in various fields of the industry such as colouring in polyester fibre, textile materials and food additives [1–8]. In addition, they have also other potential applications in science and technology as reaction initiators, fluorescent indicators, therapeutic agents, drug delivery, biosensor systems and biomedical materials [9,10]. One of the most important reasons of studying azobenzenes and its derivatives are probably to be able to adjust their properties easily and precisely [11]. Moreover, azobenzene derivatives upon photo-irradiation with UV light show isomerisation over reversal between their trans and cis forms [12–18] and resistance to thermal decomposition [19–21]. This fact enables azobenzenes to control the motion of different moities in molecules containing them [22] and so to use as a photoswitch in smart surfaces [23] and biochemical systems [24]. For instance, in biological systems, photo-induced dynamics of azo compounds changes enzyme activity and function of proteins [24,25]. Nowadays, azobenzene based-polymers have given promise in using as storage devices of optical data as consequence of significant non-linear optics feature [26–29]. For all these reasons, they have recently attracted a lot of attention in experimental and theoretical studies because of undergoing cis-trans photoisomerization in photoexcited state. Some spectroscopic and molecular structure characterizations of some azo derivatives of some 2-hydroxyacetophenone were reported previously [30]. However, novel compound "(E)-1-(5-((4-bromophenyl)diazenyl-2-hydroxyphenyl) ethanone" presente d here is a derivative of azo benzene group and providing insight into some structural properties of title compound may be of importance for researchers studying azo compounds.

In this study we present vibrational analysis of FT-IR and FT-Raman spectra by using scaled quantum mechanical procedure (SQM) of normal coordinate analysis at the density functional theory level of B3LYP/6-31G(d), and also report synthesis, results of single crystal X-ray diffraction technique and elemental analysis of this title compound.

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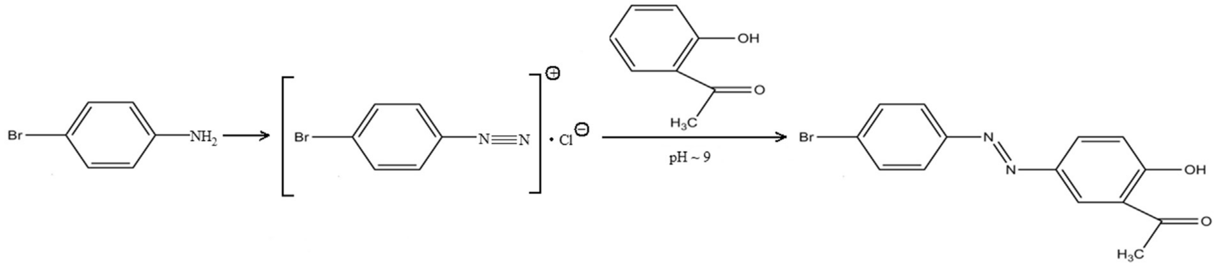

Fig. 1. Synthesis routes for the (E)-2-acethyl-4-(4-bromophenyldiazenyl)phenol.

2. Experimental

2.1. Synthesis

The 4-bromoaniline (0.860 g, 5.0 mmol), water (50 ml) and concentrated hydrochloric acid (4.7 ml, 56 mmol) were mixed and stirred until a clear solution was obtained. This solution was cooled to 273–278 K and then sodium nitrite solution (1.8 g, 26 mmol) with water was added drop by drop to this mixture while the temperature was kept below 278 K. The resulting new mixture was stirred for 30 min in an ice bath. 2-hydroxyacetofenone (0.68 g, 5.0 mmol) solution (pH 9) was gradually added to a cooled solution of 4-bromobenzenediazonium chloride, prepared as described above, and resulting mixture was stirred at 273–278 K for 60 min in ice bath. The product was recrystallized from ethyl alcohol to obtain solid (E)-2-acethyl-4-(4-bromophenyldiazenyl) phenol. The crystal of (E)-2-acethyl-4-(4-bromophenyldiazenyl) phenol was produced by slow evaporation from ethyl alcohol after one day (yield 76% m.p 457–459 K). The synthesis of compound is shown in Fig. 1. Later on, the crystal of (E)-2-acethyl-4-(4-bromophenyldiazenyl) phenol was analysed by using elemental analysis technique. As a result, C, H, O and N were found 52.72, 3.35, 10.28 and 8.69%, respectively.

2.2. X-ray diffraction analysis

Suitable single crystals were placed on a glass fibre and data collection were performed on an STOE IPDS(II) image plate detector using Mo K_α radiation ($\lambda = 0.71019$ Å) at 298 K. Furthermore, the diffraction intensities were made the Lorentz-polarisation correction factor and the absorption correction was made by integration method via X-RED software and cell parameters were found by using X-AREA software [31]. The structure was solved by direct methods using SHELXS-9722 and anisotropic displacement parameters were applied to non-hydrogen atoms in a full-matrix least-squares refinement based on F2 using SHELXL-97 [32]. All carbon and hydrogen atoms were positioned geometrically and refined by a riding model with Uiso 1.2 times that of attached atoms and remaining hydrogen atoms were found by Fourier difference. Molecular drawings were obtained using ORTEP-III [33]. Details of the crystal data, data collection conditions, structure solution and refinement are given in Table 1.

2.3. FT-IR and FT-Raman analysis

FT-IR spectrum of the compound was recorded using Bruker Optics IFS66 vs. FT-IR spectrometer with the resolution of 2 cm^{-1} in the spectral region of 4000–400 cm^{-1} with KBr pellet technique. The Raman spectrum was obtained using a Bruker Senterra Dispersive Raman microscope spectrometer with 785 nm excitation from a 3B diode laser of power 100 mW having 3 cm^{-1} resolution.

2.4. Computational procedure

The molecular structure of title compound in the gas phase was optimised by using different hybrid DFT quantum mechanical

Table 1
Crystal data, data collection conditions and structure refinement for the title molecule.

Chemical formula	$C_{14}H_{11}N_2O_2Br_1$
Formula weight	319.15
Crystal system	Monoclinic
Space group	$P2_1$
Z	2
Crystal colour	Yellow
a, b, c	4.02333(20) Å, 5.9537(4) Å, 26.7930(12) Å
β	94.182(4)°
V	640.08(6) $Å^3$
Calculated density	1.656 Mg m^{-3}
Radition, λ	Mo K_α, 0.71073 Å
μ	3.21 mm^{-1}
T(K)	296
T_{min}, T_{max}	0.4938, 0.8379
Scaning mode	STOE IPDS II
Scan range	ω
Crystal size	0.14 0.28 0.36
θ_{min}, θ_{max}	26.0° 1.5°
Number of measured/independent reflections, R_{int}	0.094
Number of reflections with 2σ(I)	2501
Number of refined parameters	172
S	0.90
R[F2 > 2σ(F2)]	0.041
wR(F2)	0.089
$\Delta\rho_{max}$, $\Delta\rho_{min}$	0.55 e $Å^{-3}$-0.23 e $Å^{-3}$

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