

Theoretical and experimental studies of newly synthesized (Z)-4-(2-(3,5-dibromo-2-hydroxy-4-methoxybenzylidene)hydrazinyl)benzonitrile compound

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ABSTRACT

(Z)-4-(2-(3,5-dibromo-2-hydroxy-4-methoxybenzylidene)hydrazinyl)benzonitrile compound (DHMB) was synthesized by a condensation reaction of 4-cyanophenylhydrazine hydrochloride and 3,5-dibromo-2-hydroxy-4-methoxy benzaldehyde. For characterization of DHMB were used IR, UV visible, LC-MS NMR devices. Kamlet-Taft and Catalan parameters were computed from max abs values obtained from UV spectra in different solvents of DMBH. It was used Gaussian 09 software for theoretical calculations. From theoretical data obtained was calculated global reactivity descriptors of DMBH.

It was observed that there was a good agreement between experimental NMR and calculated NMR data. R^2 for $^1\text{H-NMR}$ and $^{13}\text{C-NMR}$ were computed as 0.9516 and 0.8847 respectively. While parameter affecting the resolution of DMBH was solvent dipolarity parameters according to Kamlet-Taft equation, it was solvent polarizability ability according to Catalan equation.

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1. Introduction

Schiff bases are the most studied class of compounds in chemistry. There are antimicrobial activity [1–6], cytotoxicity effect [7–9], antidiabetic effect [10,11] of Schiff base and its complex. Also, it is studied sensor properties of these compounds [12–14]. Nowadays studies have shifted to investigating in the different solvents behaviours of these compounds [15–17]. Such studies help to understand in the different solvent behaviours of Schiff base compounds. Ghosh et al. [18] shown that (E)-7-(((8-hydroxyquinolin-2-yl)methylene)amino)-4-methyl-2H-chromen-2-one compound have lower fluorescence quantum yields in non-polar solvent in compared other Schiff base compounds. Tigineh et al. [19] investigated UV–vis and photoluminescence of aromatic salicylideneaniline Schiff-base in different solvent. Zhao et al. [20] worked pH induced enol-keto tautomerism of 6-(3-methoxypropylamino)pyridin-2-one based thiophene azo dyes.

In current study, (Z)-4-(2-(3,5-dibromo-2-hydroxy-4-methoxybenzylidene)hydrazinyl)benzonitrile compound (DHMB) was synthesized. Characterization of DHMB was made using different spectroscopic method. To compare experimental data,

theoretical calculations were computed via DFT B3LYP 6-311G (d,p) basis set. In order to calculate Kamlet-Taft and Catalan parameters, the UV–visible spectra were taken in different solvent. To evaluate UV–visible data was made applying multiple linear regression analysis. It was computed the global reactive descriptor and thermodynamic parameters using the data obtained from theoretical calculations.

2. Experimental section

Chemicals used in synthesis (4-cyanophenylhydrazine hydrochloride and 3,5-dibromo-2-hydroxy-4-methoxy benzaldehyde compounds) were obtained from Aldrich. Following the reaction was performed by using on a Mattson 1000 Fourier transform-infrared (FT-IR) Spectrometer in the range from 4000 to 400 cm^{-1} . NMR spectra and UV–Visible spectra were taken using on a Varian-Gemini 400 MHz spectrometer and on a Perkin Elmer lambda 35 device respectively. LC-MS spectra of DMBH was attained using by Thermo Scientific TSQ Quantum Access Max device. Synthesis scheme belong to DMBH is given below.

3. Computational details

All theoretical calculations (optimizations, IR, NMR and UV–Vis) in this study were computed via Gaussian 09 software [21].

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Visualising of results were made using GausView 5 program [22]. In theoretical computations were made DFT/B3LYP method. The 6-311G (d,p) was selected as basis set [23,24]. Theoretical NMR shift ($^1\text{H-NMR}$ and $^{13}\text{C-NMR}$) were computed within GIAO approach [25]. In NMR calculations were used as solvent DMSO. Experimental IR frequencies are different from computed IR frequencies. One of the main reasons for the difference may be that theoretical calculations are made for a single atom as well as experimental IR is taken in solid phase. To fit the theoretical data to the experimental data, theoretical IR frequencies are scaled are scaled by 0.958 [26]. VEDA 4 program was used to calculate Potential energy distribution (PED) of DMBH [27]. DOS data were calculated Gausssum 3.0 software [28].

3.1. Synthesis of DMBH

To a solution of title benzaldehyde in absolute ethanol was added 4-cyanophenylhydrazine hydrochloride (1/1). Para toluene sulfonic acid was used catalyst. Reaction process was watched disappearance of the aldehyde carbonyl peak with FT-IR Spectrometer. After the carbonyl peak disappeared, water was added to the reaction medium and the product was precipitated. Product was crystallized in absolute ethanol. Synthesis scheme of DMBH is seen in Fig. 1.

Light yellow crystal. Yield % 60, IR (KBr, ν , cm^{-1}): 3464 OH, 3279

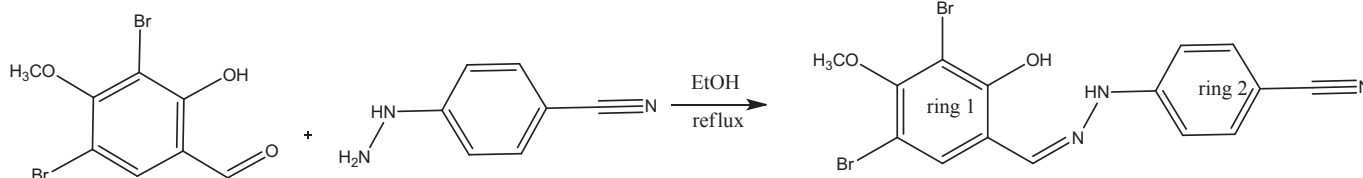


Fig. 1. Synthesis Scheme belong to the DHMB.

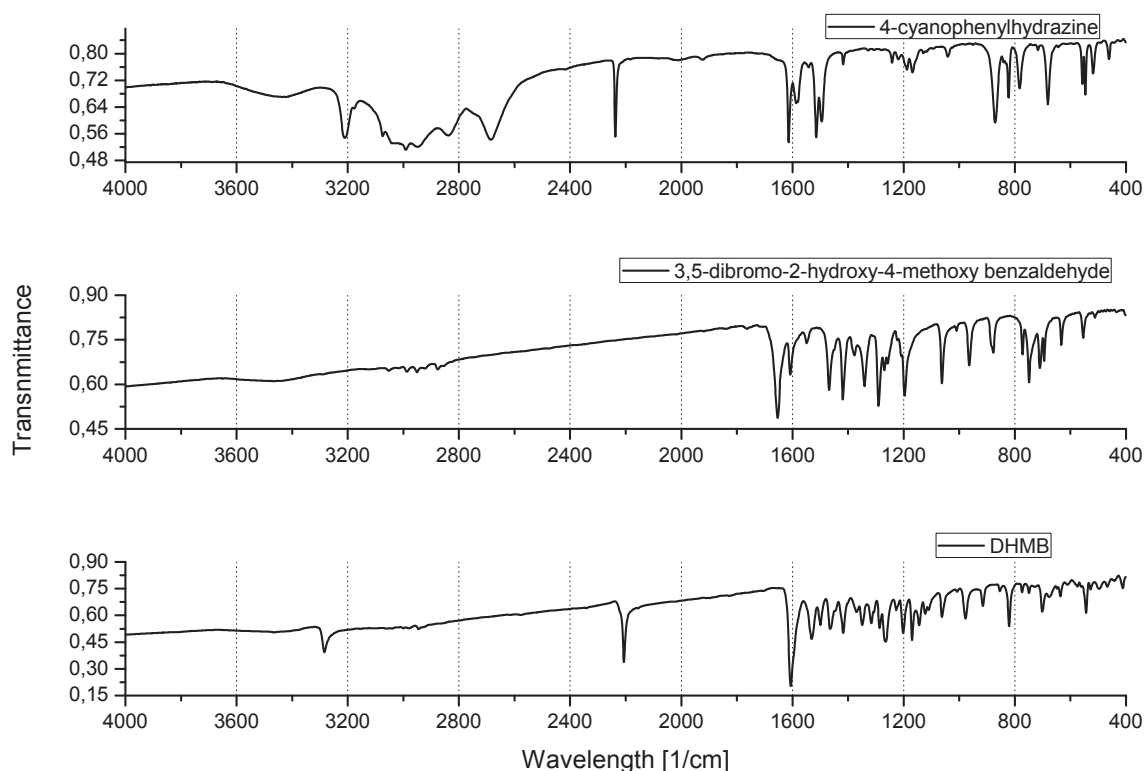


Fig. 2. FT-IR spectra for reactant and product.

NH, 2980–2945 (aliphatic C-H), 2206 ($\text{C}\equiv\text{N}$), 1606 ($-\text{C}=\text{N}-$). $^1\text{H-NMR}$ (DMSO, TMS, δ ppm): 3.81 (s, 3H, OCH_3), 7.03–7.06 (d, 2H, Aromatic, $J = 8.7$ Hz), 7.65–7.68 (d, 2H, Aromatic, $J = 8.7$), 7.85 (s, 1H, Aromatic), 8.15 (s, 1H, $\text{HC}=\text{N}$), 11.26 (s, 1H, NH), 11.37 (s, 1H, OH). m/z calculated 424.92.

4. Result and discussion

4.1. IR spectra

DHMB contain different functional groups such as OH, NH and

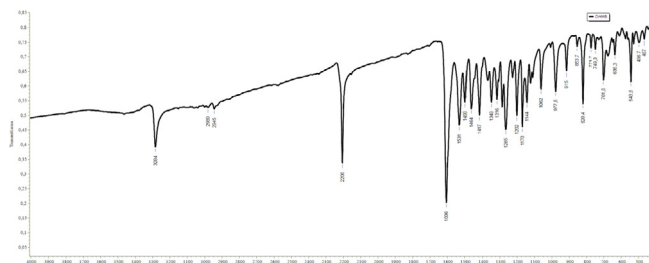


Fig. 3. FT-IR spectrum of DMBH.

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