



Molecular structure and density functional modelling studies of 2-[(E)-2-(4-hydroxyphenyl)ethyliminomethyl]phenol

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ABSTRACT

In the present work, the tautomerism in 2-[(E)-2-(4-hydroxyphenyl)ethyliminomethyl]phenol was investigated by experimental (MS, FT-IR, NMR and X-ray diffraction) and computational method [density functional theory (DFT)]. The optimized geometrical structures, atomic charges, molecular electrostatic potential (MEP), natural bond orbital (NBO) and nonlinear optical (NLO) effects of the compound have been investigated by using DFT calculations. The potential energy surface (PES) scans about three important torsion angles are performed by using B3LYP/6-311++G (d,p) level of theoretical approximation for the compound. The experimental (FT-IR) and calculated vibrational frequencies (using DFT) of the title compound have been compared. The ¹H and ¹³C NMR chemical shift assignments have been performed using DFT. To investigate the tautomeric stability, some properties such as total energy, HOMO and LUMO energies of the compound were obtained at B3LYP and B3LYP/6-311++G(d,p) level in the gas phase. The calculated results showed that the phenol-imine form of the compound was more favorite than keto-amine form. Moreover, a good correlation between experimental and theoretical data for phenol-imine form of the compound was found.

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1. Introduction

2-Hydroxy Schiff bases derived from the condensation of salicylaldehyde and 2-hydroxy-1-naphthaldehyde with various primary amines (o-OHArCH=NR₁R₂ where R₁ and R₂ represents aromatic or aliphatic groups) have gained importance day by day in present scenario. Not only have a large number of transition metal and the group 13 element complexes of 2-hydroxy Schiff bases become the topic of contemporary research in the field of coordination chemistry [1–3], but also the 2-hydroxy Schiff bases and their transition metal complexes exhibit a wide range of applications, especially in biological systems [4,5].

Two characteristic properties of 2-hydroxy Schiff bases are photochromism and thermochromism [6–9]. Their thermochromic and photochromic behaviors enable them to be utilized for the design of several molecules based on electronic devices such as

optical switches and memories, display systems, variable electrical current, ion transport through membranes and measurement of radiation intensity [10–12]. The presence of ortho hydroxyl group in 2-hydroxy Schiff bases has been regarded as one of the important elements favoring for the existence of two possible tautomeric forms, the phenol-imine and the keto-amine forms (Fig. 1). Depending on the tautomers, two types of intramolecular hydrogen bonds are observed: O–H···N in the phenol-imines and N–H···O in the keto-amines [13,14]. The appearance of these forms in 2-hydroxy salicylaldimines separately or jointly depends on the media as well as stereochemistry of the compounds and the N-substituents which provide different electron-donating or withdrawing systems [15,16]. Therefore, it has a crucial importance to investigate 2-hydroxy salicylaldimine Schiff bases by considering aforementioned factors in order to have more insight on fundamental properties of these species. The synthesis and structural research of 2-hydroxy Schiff bases derived from salicylaldehyde and 2-hydroxy-1-naphthaldehyde and amines bearing various alkyl and aryl N-substituents, as well as their metal complexes have

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