



## 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 <sup>1</sup>H and <sup>13</sup>C 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=NR<sub>1</sub>R<sub>2</sub> where R<sub>1</sub> and R<sub>2</sub> 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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# Journal Of Molecular Structure

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nucleobases and oligonucleotides peptides and proteins sugars neuromolecules non covalent complexes chiral systems interactions of low energy electrons with biomolecules in the radiation chemistry context and very large gas phase biomolecular systems The fifth chapter concerns the link between gas phase and liquid phase Different treatments of solvation are illustrated through examples pointing out the influence of progressive addition of water molecules upon properties of nucleobases peptides sugars and neuromolecules Offer a new perspective to the understanding of isolated elementary building blocks of bio molecules Includes case studies of experimental investigations coupled to quantum or classical calculations

**Molecular Structure and Spectroscopy** Henry H. Mantsch, Austin J. Barnes, 1994 Molecular Spectroscopy and Molecular Structure Austin J. Barnes, 1989 **Molecular Structures of Seven Methylenedinitramines with Plasticising Abilities**, 2002 **Molecular Spectroscopy and Molecular Structure 1991**, 1992 **Organic Chemist's Desk Reference** Caroline Cooper, Rupert Purchase, 2017-08-04 Launched in 1995 as a companion to the Dictionary of Organic Compounds the Organic Chemist's Desk Reference has been essential reading for laboratory chemists who need a succinct guide to the nuts and bolts of organic chemistry the literature nomenclature stereochemistry spectroscopy hazard information and laboratory data This third edition reflects changes in the dissemination of chemical information revisions to chemical nomenclature and the adoption of new techniques in NMR spectroscopy which have taken place since publication of the last edition in 2011 Organic chemistry embraces many other disciplines from material sciences to molecular biology whose practitioners will benefit from the comprehensive but concise information brought together in this book Extensively revised and updated this new edition contains the very latest data that chemists need access to for experimentation and research Journal of the Chemical Society Chemical Society (Great Britain), 1921 **Nitrogen Heterocycles in Cancer Therapy** Sanjeev Kumar Sahu, Ankur Vaidya, 2025-10-17 Nitrogen Heterocycles in Cancer Therapy explores the vast array of recently discovered nitrogen containing heterocyclic compounds utilized in combatting cancer This comprehensive work not only highlights the fundamentals of oncology but also explains into the intricacies of designing synthesizing and understanding the anticancer mechanisms of these compounds Spanning across 10 chapters the book explores the principles underlying the design synthesis and anticancer mechanisms of nitrogen containing heterocyclic compounds drawing from the latest research findings Its scope extends beyond molecular targeting to encompass the exploration of newly identified heterocyclic compounds with potential anticancer properties A significant emphasis is placed on crucial evaluation techniques such as in vitro cell culture and in vivo animal models providing insights into the performance of these compounds in combating cancer Particularly noteworthy is the inclusion of clinical study reports detailing the efficacy of various drug candidates across different cancer conditions coupled with an analysis of their global market impact and pharmacoeconomics Offering profound insights this book emerges as an indispensable resource for researchers clinicians and students alike offering a comprehensive understanding of the cutting edge approaches shaping the

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