



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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**Tibor Braun, H Maczelka, Andras Peter
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Molecular and Laser Spectroscopy V.P. Gupta,2017-09-18 Molecular and Laser Spectroscopy Advances and Applications provides students and researchers with an up to date understanding of the fast developing area of molecular and laser spectroscopy Editor V P Gupta has brought together the eminent scientists on a selection of topics to develop a systematic approach first covering basic principles needed to understand each cutting edge technique and application This book acts as a standard reference for advanced students of molecular and laser spectroscopy and as a graduate text for new entrants in the field The book covers a wide range of applications of molecular and laser spectroscopy in diverse areas ranging from materials to medicine and defence biomedical research environmental monitoring forensic investigations food and agriculture and chemical pharmaceutical and petrochemical processes Researchers and scientific personnel in these fields will learn the latest techniques in order to put them to practical use in their work Covers several areas of spectroscopy research in a single volume saving researchers time Includes exhaustive lists of research articles reviews and books at the end of each chapter to point readers in the right direction for further learning Features illustrative examples of the varied applications Serves as a practical guide to those interested in using molecular and laser spectroscopy tools in their research and field applications

Fullerene Research 1985: 1993 Tibor Braun,H Maczelka,Andras Peter Schubert,L Vasvari,1995-03-31 This volume contains very carefully compiled material presenting bibliographic descriptions of approximately 3500 papers with a computer generated index on authors subject headings corporate addresses and journals There are many on line services available on fullerenes but they serve mainly current awareness functions none of them is selectively complete and carefully indexed and none can replace a complete retrospective bibliography which most researchers in the field would want to have on hand in their laboratories and offices

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Handbook of High-resolution Spectroscopy Martin Quack, Frederic Merkt, 2011-09-26 The field of High Resolution Spectroscopy has been considerably extended and even redefined in some areas Combining the knowledge of spectroscopy laser technology chemical computation and experiments Handbook of High Resolution Spectroscopy provides a comprehensive survey of the whole field as it presents itself today with emphasis on the recent developments This essential handbook for advanced research students graduate students and researchers takes a systematic approach through the range of wavelengths and includes the latest advances in experiment and theory that will help and guide future applications The first comprehensive survey in high resolution molecular spectroscopy for over 15 years Brings together the knowledge of spectroscopy laser technology chemical computation and experiments Brings the reader up to date with the many advances that have been made in recent times Takes the reader through the range of wavelengths covering all possible techniques such as Microwave Spectroscopy Infrared Spectroscopy Raman Spectroscopy VIS UV and VUV Combines theoretical computational and experimental aspects Has numerous applications in a wide range of scientific domains Edited by two leaders in this field Provides an overview of rotational vibration electronic and photoelectron spectroscopy Volume 1 Introduction Fundamentals of Molecular Spectroscopy Volume 2 High Resolution Molecular Spectroscopy Methods and Results Volume 3 Special Methods Applications

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Spectroscopy and Modeling of Biomolecular Building Blocks Jean-Pierre Schermann, 2007-10-16 Spectroscopy and Modeling of Biomolecular Building Blocks presents an overview of recent advances in the intertwining of the following research fields photon and electron spectroscopy quantum chemistry modelling and mass spectrometry The coupling of these disciplines offers a new point of view to the understanding of isolated elementary building blocks of biomolecules and their assemblies It allows the unambiguous separation between intrinsic properties of biomolecular systems and those induced by the presence of their environment The first chapters provide background in modelling I frequency resolved spectroscopy using microwave infrared and UV photons time resolved spectroscopy in the femtosecond domain and energy resolved electron spectroscopy II and production of gas phase neutral and ionic biomolecular species mass spectrometry ion mobility and BIRD techniques III Chapter IV is devoted to case studies of gas phase experimental investigations coupled to quantum or classical calculations The topics are structural studies of 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 Quantitative Structure-activity Relationship Fatma Kandemirli,2017-08-30 The book which is related to QSAR in sciences is divided into five main chapters The first chapter is the Introductory chapter The second chapter aims to provide an update of the recent advances in the field of rational design of PDE inhibitors The third chapter includes designing a series of peptidic inhibitors that possessed a substrate transition state analog and evaluating the structure activity relationship of the designed inhibitors based on docking and scoring using the docking simulation software Molecular Operating Environment The aim of the forth chapter is to develop structure property relationships for the qualitative and quantitative prediction of the reverse phase liquid chromatographic retention times of chlorogenic acids The final chapter aims to determine the model of interactions between the natural compounds with anti inflammatory molecular target by molecular docking analysis *Journal of the Chemical Society Chemical Society (Great Britain),1921* Organic Chemists Compounds Desk Reference P. H. Rhodes,1991-12-31 Information from many disparate sources is brought together to create a unique desktop guide to the principles and practice of organic chemistry **The Complex World of Polysaccharides** Desiree Nedra Karunaratne,2012-10-31 The complex world of polysaccharides is a compilation of the characteristics of a variety of polysaccharides from plants animals and microorganisms The diversity of these polysaccharides arises from the structural variations and the monosaccharide content which is under genetic control The chemical and physical properties have made them useful in many pharmaceutical food and industrial applications These properties of the polysaccharides determine their biological activity and their function in various applications The role played by polysaccharides in preservation and protection of food as carriers of nutrients and drugs their ability to interact with molecules both for efficient delivery as well as improving textures of food colloids and their use as therapeutics are some of the functions discussed **Salicylic Acids—Advances in Research and Application: 2012 Edition** ,2012-12-26 Salicylic Acids Advances in Research and Application 2012 Edition is a ScholarlyEditions eBook that delivers timely authoritative and comprehensive information about Salicylic Acids The editors have built Salicylic Acids Advances in Research and Application 2012 Edition on the vast information databases of ScholarlyNews You can expect the information about Salicylic Acids in this eBook to be deeper than what you can access anywhere else as well as consistently reliable authoritative informed and relevant The content of Salicylic Acids Advances in Research and Application 2012 Edition has been produced by the world s leading scientists engineers analysts research institutions and companies All of the content is from peer reviewed sources and all of it is written assembled and edited by

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dying and paint industries as photocatalyst to improve the degradation rate Features This book would be useful for academia researchers and engineers working in the area of Schiff base and their metal complexes This book will give an in depth account of the properties of Schiff base and their metal complexes This book will discuss the details of synthesis methods for Schiff base and their metal complexes This book will cover emerging trends in the use of Schiff base metal complexes in the industry This book will provide an overview of the wider biological applications of Schiff base metal complexes

Molecular Structure and Chemical Reactivity I. G. Csizmadia, G. Herzberg, 1987

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web the tiger shark galeocerdo cuvier is a species of requiem shark and is the only member of the genus galeocerdo this is one of the largest known species of shark it reaches lengths of up to 5 5 metres 18 feet and weighs over 900 kg 2000 pounds

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web the tiger shark or galeocerdo cuvier is the last remaining member of the galeocerdo genus this apex predator is a requiem shark and it is near threatened because of fishing and finning table of contents characteristics appearance weight length tiger sharks can achieve weights of 850 1 400 pounds and lengths of 10 14 feet

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suggests they may have evolved in tandem

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web the tiger shark is a species of requiem shark that is often referred to as the sea tiger the scientific name for the tiger shark is *Galeocerdo cuvier* and it is part of the family *Carcharhinidae* there are a few different theories as to why this particular species of shark is called the tiger shark

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web tiger sharks have also become very aggressive toward spearfishermen and divers attracting the sharks in underwater photo sessions danger to humans the tiger shark like its jungle namesake is dangerous its toll of victims throughout the world is second only to that of the white shark

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web the tiger shark is one of the requiem sharks renowned as formidable predators with powerful jaws and razor sharp teeth it is the second largest predatory shark after the great white shark measuring over 5m 16ft in length and weighing 900kg 2 000 lbs

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web sep 15 2023 tiger shark *Galeocerdo cuvier* large potentially dangerous shark of the family *Carcharhinidae* it is noted for its voracity and inveterate scavenging as well as its reputation as a man eater the tiger shark is found worldwide in warm oceans from the shoreline to the open sea

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web reaching lengths of at least 18 feet 5 5 m and 2000 pounds nearly a metric tonne the tiger shark is the fourth largest shark and second largest predatory shark behind only the great white shark tiger sharks are aggressive predators famous for eating just about anything they find or are able to capture

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web oct 26 2023 the shark teeth are of a similar size and came from tiger sharks galeocerda cuvier that were approximately two metres long both teeth are perforated a complete tooth found at the cave site of

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web nov 24 2020 the tiger shark is the only member of the genus galeocerdo and is a large predatory species tiger sharks are found in many temperate and tropical oceans and are known for their distinctive stripes and spots on their flanks which resemble a tiger s stripes

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web jun 5 2018 weighing 1300 pounds or more and growing up to 15 feet the tiger shark is the fourth largest shark on earth only whale sharks basking sharks and great whites get bigger on top of

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web tiger sharks have only one recorded natural predator the orca it is considered a near threatened species because of finning and fishing by humans the tiger shark is second only to the great white in recorded fatal attacks on humans but these events are still exceedingly rare

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web what are tiger sharks tiger sharks are named for the dark vertical stripes found mainly on juveniles as these sharks mature the lines begin to fade and almost disappear shark attacks

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web the tiger shark is found in tropical and subtropical waters around the world but mostly inhabit a range between the parallels 45 north and 32 south its presence ranges from the east coast of north america to the east coast of brazil including the gulf of mexico

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web jul 15 2017 26 tiger shark teeth facts a tiger sharks tooth is uniquely shaped like the sail of a boat they are very large and notched with saw like edges 27 their teeth are so strong they can cut through the shell of a sea turtle or a clam 28 if one of their teeth break they simply grow a new one the next day 29

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