Theoretical Raman and FTIR vibrational analysis of 2-phenyl-1H-indene-1,3(2H)-dione by *ab initio* method

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Abstract. 2-phenyl-1H-indene-1,3(2H)-dione is an anticoagulant and functions as a Vitamin K antagonist. The equilibrium geometries and harmonic frequencies of the molecule under investigation was determined and analyzed at DFT level employing the basis set 6-311++G(d,p). The skeleton of the optimized molecules is found to be non-planar. The plane of the phenyl ring and the mid-plane of the bicyclic moiety are almost perpendicular to each other. In general, a good agreement between experimental and calculated normal modes has been observed. A comparison of calculated frontier orbital energy gap 2-phenyl-1H-indene-1,3(2H)-dione and 1H-indene-1,3(2H)-dione shows that the 2-phenyl-1H-indene-1,3(2H)-dione is slightly more reactive molecule than its parent. The other molecular properties of 2-phenyl-1H-indene-1,3(2H)-dione like dipole moment, polarizability, MESP potential surface have also been calculated and compared with the parent molecule.

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Key words: anticoagulant, geometry optimization, molecular electrostatic potential surface, normal mode analysis

1 Introduction

In conjunction with heparin, the use of oral anticoagulant drug therapy has become a focus of immense academic and pharmaceutical interest. Anticoagulant therapy is a course of drug therapy in which anticoagulant medications are administered to a patient to inhibit the formation of clotting agents so that the blood cannot clot easily. The drug 2-phenyl-1H-indene-1,3(2H)-dione also known as phenindione, an indandione (1H-indene-1,3(2H)-dione) derivative, has been used as an anticoagulant and functions as vitamin K antagonist. Phenindione which is a 1,3-diketone carbon acid, thins the blood and is used when the patient is allergic to warfarin [1, 2]. Pipkin, and Stella have carried out the study of tautomerism of

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phenindione, 2-phenyl-1,3-indandione, in dipolar aprotic/hydrocarbon solvent mixtures and have reported that phenindione exists predominantly in its diketo, rather than enol form in hydrocarbon solvents [3].

The aim of present communication is to investigate the molecular structural, vibrational and energetic data analysis of the molecule under study, in gas phase, due to its biological and pharmaceutical importance. The structure and ground state energy of the molecule under investigation has been analyzed by employing DFT/B3LYP level. In order to obtain more complete description of molecular motion, vibrational frequency calculation has been carried out at the DFT level. The reported geometries, molecular properties such as equilibrium energy, dipole moment, polarizability and vibrational frequencies along with electrostatic potential maps, have also been used to understand the properties of the title molecule.

2   Experimental

The model molecular structure of phenindione along with its parent molecule has been given in Fig. 1. The calculated vibrational spectra plotted in Figs. 2 and 3, has been matched with FT-IR and FT-RAMAN spectra obtained from Sigma Aldrich website [4].
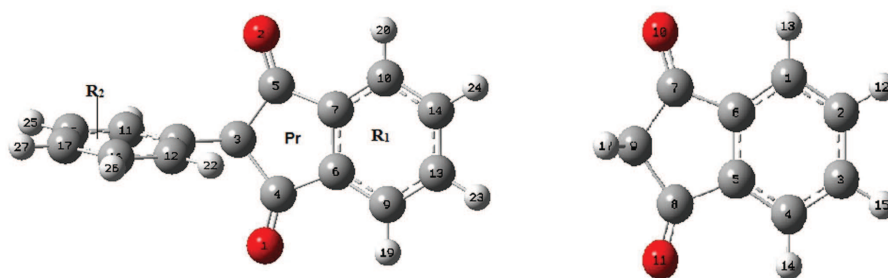

Figure 1: Optimized structure of 2-phenyl-1H-indene-1,3(2H)-dione and 1H-indene-1,3(2H)-dione.

3   Computational details

The Becke's three parameter hybrid exchange functional [5] with Lee-Yang-Parr correlation functionals (B3LYP) [6,7] of the density functional theory [8] and 6-311++G (d,p) basis set were chosen to optimize the structures of the molecules under investigation. All the calculations were performed using the Gaussian 09 program [9]. Positive values of all the calculated vibrational wave numbers confirmed the geometry to be located at true local minima on the potential energy surface. As the DFT hybrid B3LYP functional tends to overestimate the fundamental normal modes of vibrations, a uniform scaling factor of 0.9679 [10,11] has been applied and in general a good agreement of calculated modes with experimental ones has