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On the spectroscopic analyses of (E)-3-(dicyclopropyl methylene)-dihydro-4-[1-(2,5 dimethylfuran-3-yl) ethylidene]furan-2,5-dione

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ABSTRACT

In this work, a combined experimental and theoretical study on molecular structure and vibrational frequencies of (E)-3-(dicyclopropyl methylene)-dihydro-4-[1-(2,5 dimethylfuran-3-yl) ethylidene] furan-2,5-dione [DCPF] were reported. The FT-IR spectra of DCPF isomers are recorded in the solid phase. The equilibrium geometries, harmonic vibrational frequencies, thermo-chemical parameters, total dipole moment and HOMO-LUMO energies are calculated by density functional theory DFT/B3LYP utilizing 6-311G(d,p) basis set. Results showed that scaled frequencies are in good agreement with experimental values. The HOMOs and the LUMOs energies of DCPF isomers were 3.8 and 2.7 eV for E and C isomers,respectively.

1. Introduction

Organic photo-chromic compounds are considered as promising candidates for application in photo-switchable systems [1–4], spatial light modulator, optical wave guide component, high density optical storage, holographic phase conjugators and finally in optical memory devices [5–7]. (E)-3-(dicyclopropyl methylene)-dihydro-4-[(1-(2, 5 dimethylfuran-3-yl) ethylidene]furan-2,5-dione which is termed as DCPF has a chemical formula of $C_{19}H_{20}O_4$. DCPF is belonging to a class of compounds called fulgides [6]. It shows a complete reversible photo-chromism with minimum photochemical fatigue [2,8], thermal stability [9] and non-destructive readout stability [2,7]. The optical properties of vacuum deposited thin films of DCPF are studied [10]. It is stated that, the photochromic properties of films are lost as a result of annealing. The dielectric constant, oscillator energy and dispersion energy slightly increase upon conversion from E- to C-isomer. Nowadays a novel series of fulgides based on different heterocycles such as furan, thiophene, pyrrole a well as many other heterocycles are obtained and studied extensively [11–13]. In spite of this it is worth to mention that experimental and/or molecular modeling studies for the molecular structure of DCPF isomers are still limited. Molecular modeling was utilized beside FTIR for studying the molecular structure of many systems and structures [14–18]. Accordingly, in the present work both experimental and molecular modeling is combined for studying the optimized molecular structural parameters, vibrational spectra, thermodynamical parameters, total dipole moment and HOMO-LUMO energies for E and C isomers using Density Functional Theory DFT/B3LYP utilizing 6-311G(d,p) basis set.

2. Experimental details

2.1. Sampling

The DCPF was prepared in powder form following Stobbe condensation method [19]. The powder was re-crystallized using ethanol then the E isomer is obtained as yellow crystals. The C isomer was obtained by irradiating E isomer thin film with UV light for 15 min. Both the E and C Isomerization Pathway of DCPF is indicated in Fig. 1.

2.2. Instrumentations

For the irradiation of E isomer the Black Ray UV L21 system of wavelength 366 nm was used.

For X-ray single crystal the preliminary examination and data collection were performed with Mo Kα radiation (λ = 0.7107 Å) on an automatic Kappa CCD single crystal diffraction (Enraf Nonious FR59) computer controlled system, equipped with graphite crystal monochromator installed in the path of incident beam. The data were collected at room temperature (298 K) and from θ_{min} = 2.91° to

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