Available online at **www.joac.info**

ISSN: 2278-1862

Journal of Applicable Chemistry

2016, 5 (2): 346-368

(International Peer Reviewed Journal)

FT-IR, FT-Raman and UV-Visible Analysis of (2E, 6E)-2, 6-Dibenzylidene-4-(4-Hydroxyphenyl) Cyclohexanone-DFT Method

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Accepted on 17th February 2016

ABSTRACT

FT-IR, FT-Raman and UV-Visible spectra of (2E,6E)-2,6-dibenzylidene-4-(4-hydroxy phenyl) cyclo hexanone (DHC) was recorded in the regions of 4000-400 cm^{-1}, 3500-50 cm^{-1} and 200-800 nm, respectively. The geometrical parameters and harmonic wavenumbers were calculated using DFT/B3LYP/6-31G (d,p) level of basis set. The NLO behavior of the title molecule was measured using first order hyperpolarizability calculation. Hyperconjugative interaction and charge delocalization have been analyzed. The calculated HOMO-LUMO energy gap shows the stability of the molecule. Molecular electrostatic potential (MEP) was studied for predicting the reactive sites. Mulliken charges were also calculated. The theoretical IR, Raman and UV-Visible spectra of DHC have also been constructed and correlated with the experimental results.

Keywords: Cyclohexanone, synthesis**,** FT-IR, DFT, NLO, NBO, UV, NMR analysis.