Synthesis, Molecular Structure, HOMO-LUMO and Spectroscopic Investigation of (*E*)-1-(2,4-Dichloro-5-fluorophenyl)-3-(2,6-dichlorophenyl)prop-2-en-1-one: A DFT Based Computational Exploration

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Abstract

In present study, the synthesis, molecular structure, HOMO-LUMO and spectroscopic investigation of (*E*)-1-(2,4-dichloro-5-fluorophenyl)-3-(2,6-dichlorophenyl)prop-2-en-1-one (CFPCP) is reported. The structure of the title compound was affirmed based on FTIR, ^{1}H NMR & ^{13}C NMR spectroscopic techniques. The computational examination has been performed by employing density functional theory (DFT) method at B3LYP/6-311G++(d,p) basis set. The geometry of the title molecule has been optimized and established at the same level of theory. The various structural and quantum chemical parameters have been investigated for the title molecule at the 6-311G++(d,p) basis set. To explore the electron distribution, Mulliken atomic charges and molecular electrostatic potential surface are discussed. Besides, vibrational assignments were made and the scaled frequencies have been compared with the experimental frequencies. For the investigation of the absorption wavelength, excitation energy and the oscillator strength TD-DFT method using B3LYP/6-311G++(d,p) basis set is used. Some thermochemical functions have also been investigated using harmonic vibrational frequencies.

Keywords

(*E*)-1-(2,4-Dichloro-5-fluorophenyl)-3-(2,6-dichlorophenyl)prop-2-en-1-one, DFT, 6-311++G(d,p), FMO.

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