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Synthesis, Thermo-Optical Characterization, Crystal Structure, Hirshfeld Surface Analysis and DFT Studies Of ((4-Chloro-6-Methyl-2-Oxo-2H-Chromen-3-Yl) Methylene) Benzene-Sulfonohydrazide

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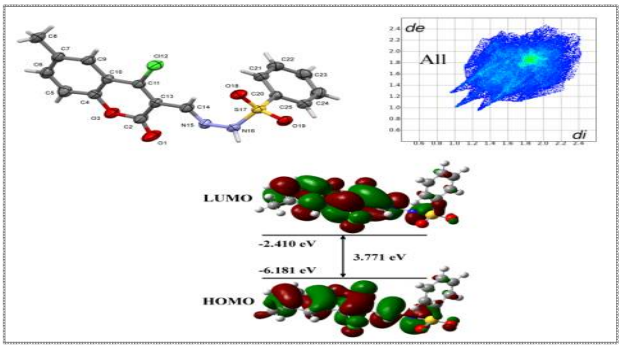
ABSTRACT

The coumarin derivative ((4-chloro-6-methyl-2-oxo-2H-chromen-3-yl) methylene) benzene-sulfono-hydrazide was synthesized by condensation reaction, characterized by spectroscopic techniques (^{1}H NMR, ^{13}C NMR, FTIR, UV-Vis, TGA and DSC) and finally the structure was confirmed by X-ray diffraction method. The thermal studies showed that the title compound is thermally stable up to 200°C and they undergo endothermic decomposition at higher temperatures. The crystal structure revealed that the compound crystallizes in $P\bar{1}$ space group. The compound exhibits diverse intermolecular interactions including C-H…O, N-H…O, C-H…Cl type of hydrogen bonds, C-Cl…Cg and Cg…Cg interactions. The molecules form alternative $R_2^2(14)$ and $R_4^4(20)$ supramolecular synthons through intermolecular hydrogen bonds which connect them to an infinite one-dimensional chain along [0 11] direction. The Hirshfeld surface analysis showed that H…H (29.4%) and O…H (28.7%) are the major intermolecular interactions. Further the structure was optimized using density functional theory (DFT) calculations. The optimized geometrical parameters show very good agreement with those determined by XRD method. The time dependent density functional theory (TDDFT) calculation was used to study electronic transition among the first 15 molecular orbitals. The calculated electronic absorption spectrum compliments the experimentally measured UV-Vis spectrum.

Graphical Abstract



Keywords: Coumarin-sulfonylhydrazide, Crystal Structure, UV-Visible, Density Functional Theory.