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Crystal Structure, Hirshfeld Surface Analysis, Energy Frameworks and DFT Studies of 1-methylindoline-2, 3-Dione

S. R.Kumar Swamy[1], M. K.Hema[2], Mahesha[2], K. J.Pampa[3] and N. K.Lokanath[2]*

1. Department of Physics, Maharani's Science College for Women, Mysuru-570005, **INDIA**
2. Department of Studies in Physics, University of Mysore, Manasagangotri, Mysuru-570 006, **INDIA**
3. Department of Studies in Biotechnology, University of Mysore, Manasagangotri, Mysuru-570 006, **INDIA**

Email: lokanath@physics.uni-mysore.ac.in

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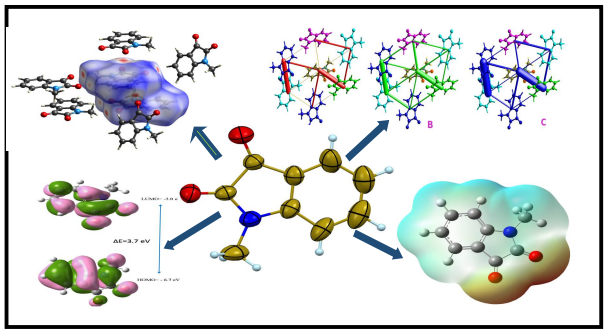
ABSTRACT

Isatin derivative, 1-methylindoline-2,3-dione single crystals were grown by slow evaporation method using methanol solvent and the structure was determined by single crystal X-ray diffraction. The title compound is crystallized in the monoclinic space group $P2_1/c$, which exhibits various intra and intermolecular hydrogen bond interactions along with C-H…Cg and Cg…Cg interactions. Intermolecular hydrogen bond interactions C9A-H2B...O2B and C4A-H16…O1B combines to form supramolecular ring motif $R_2^2(11)$ along crystallographic ab plane. Hirshfeld surface analysis revealed that C-H…O(30.4%), H…H(25%) and C-H(18%) interactions are dominantly contribute in the crystal packing leading to the structural stability. Further the coordinates were optimized by DFT calculations with basis set of 6-311+G(d,p).The optimized structural parameters showed very good correlation with those determined by XRD method. The Mulliken charge, molecular electrostatic potential map, frontier molecular orbitals were investigated and the HOMO and LUMO energy gap was found to be 3.7 eV. The interaction energies were also calculated and energy frames were explored using Crystal Explorer, which confirm that the dispersion energy framework is dominant over the electrostatic energy frameworks.

Graphical Abstract



Keywords: Crystal structure, Hirshfeld surface, Energy frameworks, DFT calculation.