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Synthesis, Characterization and Theoretical Study of 3-(4-bromophenyl) -5-(2,4-dichlorophenyl)-1-phenyl-4,5-dihydro-1*H*-pyrazole

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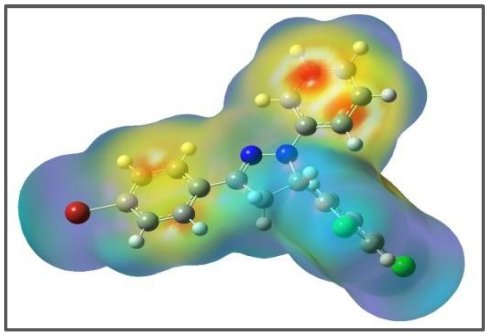
ABSTRACT

The 3-(4-bromophenyl)-5-(2,4-dichlorophenyl)-1-phenyl-4,5-dihydro-1H-pyrazole (BCPP) was synthesized from chalcone. The optimized geometrical parameters and vibrational spectra of BCPP have been investigated by Density Functional Theory (DFT) using B3LYP method at 6-311++G(d,p) basis set with Gaussian-03(W) package. Structural parameters such as atomic charges, bond lengths, bond angels, dipole moment, molecular electrostatic potential, HOMO-LUMO energies and various thermochemical parameters of titled compound also investigated with same level of theory. Experimental FT-IR vibrational frequencies have been analyzed and compared with theoretically predicted vibrational frequencies.

Graphical Abstract



MEP diagram for BCPP

Keywords: Chalcone, DFT, HOMO-LUMO, FT-IR.