Structure Analysis, Vibrational Spectral Properties, Thermodynamic Properties, and Frontier Molecular Orbital Analysis of 4-(Difluoromethoxy) Benzaldehyde by DFT

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ABSTRACT

Substituted benzaldehydes are simple aromatic compounds and their derivatives are widely used in different industries such as dyes, flavouring, artificial flavours, solvents, etc. they also exhibit different biological activities. Due to these reasons, there exists a vast scope of study of substituted benzaldehydes, in this light4-(difluoromethoxy) benzaldehyde is reported for the study. The experimental values of IR and Raman spectra for different assignments studied by earlier researchers are compared with those obtained by the Gaussian 09W program package using the Becke-3Lee-Yang-Parr (B3LYP) functional supplemented with the standard 6-31G (d,p). The thermodynamic properties are discussed with the different thermodynamic constants obtained in the temperature range 200K-1500K. Frontier molecular orbits (HOMO-LUMO) and molecular electrostatic potentials (MESP) are also studied.

Keywords: Substituted benzaldehydes, Vibrational Spectral studies,4-(difluoromethoxy) benzaldehyde Studies, Gaussian 09W, HOMO-LUMO, Frontier Molecular Orbitals.