Physico-Chemical Properties and DFT Calculations of Cuminaldehyde Using Gaussian Basis Set

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ABSTRACT

Physico-chemical properties play an important role in determining the toxicity of a material Gaussian 09, the software package was used for the theoretical quantum chemical calculations of Cuminaldehyde, DFT/B3LYP/6-311G (d, p) basis was used to perform geometric optimization and vibrational frequency determination of the molecule. The statistical thermochemical calculations of the molecule were done at DFT/B3LYP/6-311G (d, p) basis set to calculate the standard thermodynamic functions: heat capacity (CV), entropy (S), and Enthalpy (E). UV-Visible absorption spectra, ECD spectra, electronic transitions, vertical excitation energies, and oscillator strengths of Cuminaldehyde were computed by Time-Dependent DFT (TD-DFT) method using the same basis set. FMO analysis, Molecular electrostatic potential study was also done using the same basis set.

Keywords: Physico-chemical property, Gaussian 09 software, DFT, Cuminaldehyde, FMO.