Vibrational Spectral Studies, Thermodynamic Properties, And Molecular Orbital Analysis of 4-Methoxybenzaldehyde (p-Anisaldehyde) By D F T

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ABSTRACT

Benzaldehyde is best known as being artificial essential oil of almonds and it has many other uses such as; the manufacturing of dyes, perfumes, flavourings, cinnamic and mandelic acids, and it is also used as a solvent. Some more recent developments in the use of benzaldehyde are for the health and agriculture industries. Due to these basic reasons, there exists a vast field of study on substituted benzaldehydes. The optimized geometry, frequency, and intensity of the vibrational bands of 4-Methoxybenzaldehyde were obtained by Density Functional Theory (DFT) using Gaussian 09 software package. Thermodynamic properties and molecular orbital were analysed.

Keywords: Benzaldehydes, Vibrational spectral studies, 4-Methoxybenzaldehyde, DFT, Gaussian 09.