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Breakthrough Research and Technologies in Physics for a Sustainable Future

Koyel Ganguly
Soumyadipta Pal
Kamakhya Prasad Ghatak
Editors

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Contents

Chapter 7

DFT-Based Analysis of Toxic VOCs to Evaluate Their Structural Stability and Sustainability

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Abstract

This study describes the electronic properties of two industrially important VOCs, categorised as toxic pollutants, namely ethane and toluene. Density Functional Theory (DFT) calculations were performed on both compounds using Gaussian 09W and GaussView 6.0, with an emphasis on key electronic parameters. It covered the molecular orbitals (MOs), molecular electrostatic potential (MEP), band structure, infrared (IR) spectra and electron localisation function (ELF). From IR spectra analysis, it was found that the symmetry was much higher in ethane than in toluene. The energy gap for molecular orbitals was obtained as +0.452 Hartree for ethane and +0.241 Hartree for toluene. Ethane was chosen here due to its widespread presence in industrial processes and natural gas, making it a relevant baseline for comparative analysis. Toluene, on the other hand, is a more toxic aromatic compound commonly found in solvents and fuel emissions, necessitating closer investigation of its electronic properties. It presents an essential study on the identification and detailed characterisation of these toxic VOCs, which is crucial for

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