

ABSTRACT

Computational models are very important in understanding the nature of interactions in chemical systems from which important geometry parameters for various organic compounds can be extracted. This study explores computationally the geometry parameters of selected volatile organic compounds from the co-pyrolysis of Croton megalocarpus biodiesel blend using the Density functional theory (DFT) in conjunction with B3LYP correlation function at 6 - 31 G basis set. Gaussian '16 computational and Chemissian version 4.43 computational codes were used to generate electron density maps, band gap energies and frontier molecular orbitals. Frontier orbitals are central in estimating the reactive nature of a given molecular compound. The results indicated that the thermal degradation of selected molecular products from the co-pyrolysis of Croton megalocarpus biodiesel blends proceeds via high energy barriers between 400 and -1250 kJ/mol. Fundamentally the highest occupied and the lowest occupied molecular orbitals (MOs) are critical in determining the reactivity of a molecule. Moreover, the HOMO-LUMO band gap energies of 4-(2,4-dimethylcyclohexyl)-2-butanone, 3,4-dimethyl-3-cyclohexene-1-carbaldehyde, 5-(3-phenylpropanoyl) dihydro-2(3H)-furanone, and isopropenyl-4-methyl-1,2-cyclohexanediol were 0.674 eV, 3.918 eV, 3.393 eV, and 1.588 eV, respectively.

Keywords

Optimization, Band Gap, Density Maps, Mechanisms