Thermodynamic analysis of Biobutanol via DFT

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Abstract

This work has the purpose of carrying out a theoretical survey of the thermodynamic properties of Biobutanol with its isomers, in order to evaluate its thermodynamic potential as complementary fuel or even substitute for ethanol and gasoline, thus contributing to the reduction in the emission of pollutant gases to the atmosphere. For this, Gaussian09W software was used to perform molecular geometry optimization calculations using DFT with B3LYP hybrid functional, functional and the base set 6-31 G (d,) to obtain the second energy minimization of the molecular geometries. After the molecular optimization step, the fundamental frequency calculations of the molecules were performed, where the molecular vibration modes for the frequencies were obtained. In order to perform the frequency calculations, the same functional parameters and set of bases previously mentioned for the optimization were used. The results obtained by the simulated in Gaussian09W correspond to the thermodynamic properties of each of the molecular components of the fuels discussed in this work. These properties were: the specific molar heat at constant volume, enthalpy of formation, entropy and free energy of Gibbs. All simulations were repeated for temperatures in the range of 100K-1500K and constant pressure of 1atm, in order to obtain data on how thermodynamic properties behave as a function of temperature.

Keywords: Bioutanol, thermodynamic properties, DFT.