Título: THERMODYNAMIC DFT OF NEW BIOFUELS

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Abstract: We purpose simulation of new biofuels as inflammable molecules (alcohols and ethers), in order to evaluate its thermodynamic properties of these new fuels using DFT with B3LYP hybrid functional and the base set 6-31 G(d) to perform energy minimization of the molecular geometries and frequency calculations. The results obtained by Gaussian 09W of each of the molecular components of the fuels discussed in this work are comparable with experimental results of literature or measure by us. These properties were the specific molar heat at constant pressure, enthalpy of formation, entropy and free energy of Gibbs in the temperature range of 10K-700K at 1 atm, in order to obtain thermodynamic properties behavior as a function of temperature.

Keywords: thermodynamic properties, New biofuels, DFT.