DFT and canonical calculation for the thermodynamic Analysis of Gasoline Additives: ETBE, MTBE, DIPE, Ethanol and Methanol

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Abstract

A physical-chemistry analysis was performed with Density Functional Theory and a canonical ensemble, to predict the thermodynamic properties of gasoline with additives at the gas phase. These calculated quantities included a standard gasoline type mixed with the following oxygenate additives: methyl tert-butyl ether, ethyl tert-butyl ether, di-isopropyl ether, ethanol and methanol. For each gasoline and additive mixture, thermodynamic potential variations (enthalpy, entropy and Gibbs free energy) were calculated which respect to their combustion, where an analysis of the additive effect was performed to estimate relevant fuel properties for this burning process. Thus, we observed that alcohol additives presented the least expressive values of standard Gibbs free energy, rendering their gasoline combustion less favorable to the combustion, while the ester additives did not significantly alter this quantity in the gasoline. Then, it may be seen that ethanol and methanol have the capacity to make the heating of this fuel less favorable to the burning, acting as antiknock additives, enabling a better consumption of the gasoline when injected into the combustion chamber.

Key-words: Additives of gasoline; DFT; Thermodynamic Properties.