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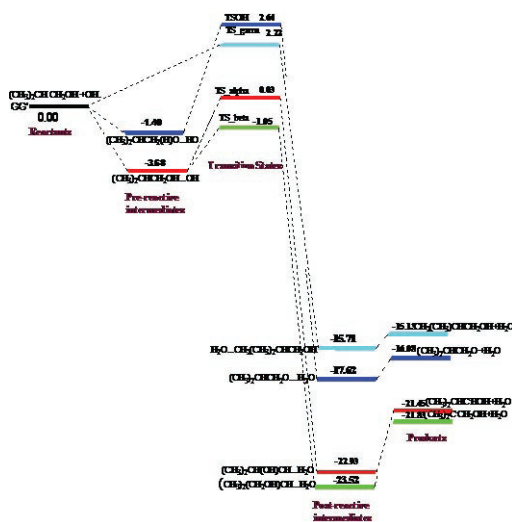
Thermochemistry and kinetics of bioalcohols and bioesters as fossil fuel alternatives Ab initio and DFT studies

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Our concern is devoted to biofuel derived from non-food crops (second-generation biofuel). Accurate thermodynamic and kinetic parameters are needed for detailed mechanism of combustion of fuel. Computational chemistry represents a valuable tool for getting such parameters. The calculations have been performed using ab initio (CCSD(T) and CBS-QB3) and Density Functional Theory (DFT) (BMK, B3LYP) procedures.

Rate constants and branching ratios for decomposition of bioalcohols and bioesters have been calculated. For 2-butanol, the results indicated that the dehydration to 1- and 2-butene through four-center transition states is the most dominant channel at low to moderate temperatures ($T \leq 700$ K). The formation of such butenes is kinetically and thermodynamically more favorable than other complex and simple bond scission reactions. Although the C-C bond fission channels require more energy than needed for some complex decomposition reactions, the former pathways predominate at higher temperatures ($T \geq 800$ K) due to the higher values of the pre-exponential factors.

Isobutanol is oxidized with the OH radical through low energy barriers of -1.0– 2.64 kcal/mol. Rate constants and branching ratios show H-abstraction from C α as the dominant reaction over the whole temperature range of 200–2000 K, with a competition from C β channel at lower temperature up to 600 K. The data obtained reproduce the available experimental findings with good performance of DFT B3LYP method compared to high ab initio levels.



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