Molecular simulation studies on chemical reactivity of methylcyclopentadiene

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ABSTRACT

Molecular simulations are important to predict thermodynamic values for reactive chemicals especially when sufficient experimental data are not available. Methylcyclopentadiene (MCP) is an example of a highly reactive and hazardous compound in the chemical process industry. In this work, chemical reactivity of 2-methylcyclopentadiene, including isomerization, dimerization, and oxidation reactions, is investigated in detail by theoretical computational chemistry methods and empirical thermodynamic–energy correlation. On the basis of molecular simulations, an average value of -15.2 kcal/mol for overall heat of dimerization and -45.6 kcal/mol for overall heat of oxidation were obtained in gaseous phase at 298 K and 1 atm. These molecular simulation studies can provide guidance for the design of safer chemical processes, safer handling of MCP, and also provide useful information for an investigation of the T2 Laboratories explosion on December 19, 2007, in Florida.