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Examination of the potential energy surface of the alkanes iodation reaction on the basis of density functional theory

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Abstract

Thermodynamic parameters of free-radical iodating of alkanes by *tret*-butylhypoiodite in gas phase and in solutions with the help of calculations by density functional method with the use of full electronic base set DGDZVP have been analyzed. Thermodynamic feasibility for iodating of saturated hydrocarbons *t*-BuOI has been shown. Transition states, activation energies, and velocity constants for basic stages of radical iodating of methane by *tret*-butylhypoiodite have been calculated. Contribution of polyvalent iodine compound $(t\text{-BuO})_3\text{I}$ into the process of iodating has been discussed.