THEORETICAL STUDY OF DIMERIZATION KINETICS OF ALUMINUM OXIDE

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Abstract: The study is aimed at the quantum chemical investigation of alumina dimerization. The appropriate potential energy surface is explored using the hybrid density functional with perturbative second-order correlation B2PLYP. It is shown that the interaction of two Al_2O_3 monomers leads to $(Al_2O_3)_2$ formation in different forms. The RRKM-based analysis revealed that the rate constant of $2Al_2O_3 \rightarrow (Al_2O_3)_2$ process can be lower by several orders of magnitude than the estimates by the rigid-sphere theory. The corresponding temperature- and pressure-dependent rate constant can be expressed by the Lindemann fit as follows: $k_0(T) = 8.01 \cdot 10^{19} T^{-1.079} \exp(21671/T)$ cm^6/(mole^{2}s) and $k_\infty(T) = 9.91 \cdot 10^{19} T^{-1.754} \exp(-2911/T)$ cm^3/(mole·s).

Keywords: alumina; dimerization; RRKM

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