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 Al₂O₃ monomers leads to (Al₂O₃)₂ formation in different forms. The RRKM-based analysis revealed that the rate constant of 2Al₂O₃ → (Al₂O₃)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: 

\[ k_0(T) = 8.01 \times 10^{19} T^{-1.079} \exp(21671/T) \text{ cm}^6/\text{(mole}^2\text{s}) \] 

and 

\[ k_{\infty}(T) = 9.91 \times 10^{19} T^{-1.754} \exp(-2911/T) \text{ cm}^3/\text{(mole} \cdot \text{s}) \]

Keywords: alumina; dimerization; RRKM

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References


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