

Quantum chemical study of mechanisms of the reaction of cyclohexyl phenyl sulfide with water

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Abstract

© 2015 Springer Science+Business Media New York. Some possible reactions of cyclohexyl phenyl sulfide with water are examined. Cyclohexyl phenyl sulfide was chosen as a model compound of heavy oils. Quantumchemical calculations of the difference in the energy of the products and reagents and the energy barrier of the reactions are performed and the temperature dependence of the change in Gibbs energy free energy is determined. It is shown that the data obtained using the density functional theory agree with the experimental data and could be used for more detailed study of the mechanisms of aquathermolysis reactions, including catalytic effects.

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Keywords

Aquathermolysis, Density functional theory, Gibbs energy, Heavy oil