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化学

甲烷的氢同位素交换的热力学理论计算

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摘要 〖HTSS〗应用密度泛函理论（DFT）/B3LYP/6 31G ** 方法计算了甲烷的氢同位素交换的各反应标准摩尔生成焓、标准摩尔生成熵、标准摩尔吉布斯自由能和平衡常数。计算结果表明，温度是影响反应热力学的重要因素，较高温度有利于甲烷的氢同位素交换，但温度太高将有较多的积炭生成，欲得到较高的转化率，需要一合适的反应温度。

关键词 甲烷；氢同位素交换；密度泛函理论

分类号

Thermodynamic Investigation on Methane of Hydrogen Isotope Exchange

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Abstract The standard enthalpy, standard entropy, standard Gibbs free energies and equilibrium constants of reactions concerned in methane of hydrogen isotope exchange were calculated with the density functional theory (DFT) using B3’ exchange and Lee Yang Parr’s correlation functional (B3LYP) with 6 31G ** basis set. The temperature is the key factor which affects the reaction thermodynamics. The higher temperature is propitious for the methane of hydrogen isotope exchange, however, the more carbon deposit is produced if the temperature is too high. A suitable reaction temperature is prerequisite for obtaining a higher yield.

Key words methane hydrogen isotope exchange density functional theory

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