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论文

溶剂化效应对6-亚甲基环戊二烯酮与HCN的反应机理影响的理论研究

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摘要:

在B3LYP/6-311+G**计算水平上, 采用导体极化连续模型研究了溶剂化效应对6-亚甲基环戊二烯酮与HCN反应生成主要产物b类酸的反应机理的影响. 计算结果表明, 在溶剂中的反应机理与在气相中的反应机理一致. 溶剂化效应使反应路径中各驻点的自由能降低, 稳定化了各物质. 溶液中的活化自由能与气相相比也有所降低, 反应更容易发生, 其中CC进攻方式的活化自由能降低得更多.

关键词: 6-亚甲基环戊二烯酮 HCN 导体极化连续模型 溶剂化效应

Theoretical Study of Effect of Solvent on the Mechanism of Reaction of Pentafulvenone with Hydrocyanic Acid

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Abstract:

Theoretical investigation of the solvent effects on the mechanism of the reaction of pentafulvenone with hydrocyanic acid to produce the main product of acid of type b was carried out at B3LYP/6-311+G** level *via* the conductor-like polarizable continuum model(CPCM). The calculation results show that the reaction mechanism in solvent is consistent with that in gas phase. The free energies of each point in channel decrease, which was caused by the solvent effects. The solvent effects stabilize each species. The activating free energies in solution phase fall down, which was comparative to that in gas phase. The reaction proceeds easier and the activating free energies decrease more in the CC attacking channel.

Keywords: Pentafulvenone HCN Conductor-like polarizable continuum model Solvation effect

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