有机化学 2000 20 (4): 587-590 ISSN: 0567-7351 CN: 31-1320/06

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· 王大喜

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多胺基烷基酰胺生成机理的量子化学研究

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收稿日期 修回日期 网络版发布日期 接受日期

摘要 用量子化学方法研究了丙酸与多乙烯多胺缩合反应机理。采用AM1方法全优化计算了丙酸多胺盐及其质子化盐的几何构型、电子结构以及酸催化下的亲核加成和消除反应的机能曲线，求得该两步反应的活化能分别为6.258kJ/mol和206.15kJ/mol。消除反应是速度控制步骤。发现质子化后丙酸羰基碳原子上的净电荷增大，前线分子轨道能级差减小，前线分子轨道间相互作用增强，表明酸催化大大增强反应活性。

关键词 酰胺P 丙酸 缩合反应 反应机理 活化能 多乙烯多胺 几何异构 电子结构

分类号 0641

Quantum chemistry applied to condensation mechanism of formation of alkyl polyethyleneamide

Wang Daxi,Wang Zhaohui

Abstract Quantum chemistry is applied to the study of condensation mechanism of the reaction between propionate acid and polyethylene polyamine. It is found that the activation energy is increased remarkably by acid catalyst. Nucleophilic addition and elimination are considered as the key steps of this reaction, and the rate of reaction is determined by the latter. By using AM1 method, equilibrium geometries, net charges and the potential curves of the reaction are obtained. The activation energies calculated for the nucleophilic addition and elimination are 6.258kJ/mol and 206.15kJ/mol respectively. The results indicate that protonation of O(3) atom lead to an increase of charge on C(2), N(12) and smaller gap between the HOMO and LUMO. This suggests the interaction between the frontier orbitals is enhnced by protonation. In this case, acid catalyst plays an important role in the reaction.

Key words AMIDES P PROPIONIC ACID CONDENSATION REACTION REACTION MECHANISM ACTIVATION ENERGY GEOMETRICAL ISOMERISM ELECTRONIC STRUCTURE

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