高等学校化学学报 2006, 27(4) 680-683 DOI: ISSN: 0251-0790 CN: 22-1131/O6

论文

三聚氰胺和环三酮氢键复合物的理论研究

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摘要:

用AM1和PM3方法对三聚氰胺和环三酮衍生物的超分子复合物进行理论研究, 得到稳定化能和相对生成焓; 在AM1优化构型的基础上, 分别用INDO/SCI和AM1方法计算复合物的电子光谱和红外光谱. 结果表明, 两个单体通过氢键形成多聚体, 导致体系能量降低, 单体的电性和位阻差异能改变体系的稳定化能. LUMO-HOMO能隙的减小使电子光谱吸收峰发生红移, 氢键的形成削弱了单体原来的N—H键, 使红外振动频率变小.

关键词: 三聚氰胺; 环三酮; 氢键; 半经验计算

Theoretical Studies on Hydrogen bonding Complexes of Melamine and Cyclotrione

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Abstract:

Supermolecular complexes of melamine and cyclotrione derivatives were studied with AM1 and PM3 methods and the stabilization energy and relative enthalpy of formation were obtained. Electronic spectra and IR spectra of complexes were calculated by using INDO/SCI and AM1 methods based on AM1 geometries. It is indicated that the monomers form the dimmer via hydrogen bonds, leading to the decrease of total energy in the system, and electronegativity and steric effects of the substituents affect stabilization energy. UV absorptions of the complexes are red shifted compared with those of the monomers owing to the less LUMO-HOMO energy gap. IR frequencies of N—H bonds in the complexes are lessened due to the formation of hydrogen bonds.

Keywords: Melamine; Cyclotrione; Hydrogen bonding; Semi empirical calculation

收稿日期 2005-04-28 修回日期 网络版发布日期 2006-04-10

DOI:

基金项目:

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