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研究论文

NTO二聚体分子间相互作用的理论研究

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摘要 在DFT-B3LYP/6-311＋＋G**水平上求得NTO二聚体势能面上六种优化构型和电子结构. 经基组叠加误差(BSSE)和零点能(ZPE)校正, 求得分子间最大相互作用能为－53.66 kJ/mol. 二子体系间的电荷转移很少. 由自然键轨道分析揭示了相互作用的本质. 对优化构型进行振动分析, 并基于统计热力学求得200.0～800.0 K温度范围从单体形成二聚体的热力学性质变化. 发现二聚主要由强氢键所贡献, 但结合能大小并不为氢键所完全决定. 二聚过程在较低温度或常温下能自发进行.

关键词 3-硝基-1,2,4-三唑-5-酮(NTO) 分子间相互作用 密度泛函理论 自然键轨道分析 热力学性质

分类号

Theoretical Study on Intermolecular Interactions of 3-Nitro-1,2,4-triazol-5-one Dimers

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Abstract Six optimized stable NTO dimers found on the potential energy surface and their electronic structures have been obtained by using density functional theory method at the B3LYP/6-311＋＋G** level. The intermolecular interaction energy was calculated with basis set superposition error correction and zero point energy correction. The greatest corrected intermolecular interaction energy of the dimer is －53.66 kJ/mol. Charge transfer between two subsystems is small. Natural bond orbital analysis was performed to reveal the origin of the interaction. Based on the vibrational analysis, the changes of thermodynamic properties from the monomer to dimer with the temperature ranging from 200.0 to 800.0 K have been obtained using the statistical thermodynamic method. It was found that the strong hydrogen bonds contribute to the dimers dominantly, while the binding energies are not only determined by hydrogen bonding. The dimerization process can occur spontaneously at lower or room temperature.

Key words 3-nitro-1 2 4-triazol-5-one intermolecular interaction density functional theory natural bond orbital analysis thermodynamic property

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