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Full Paper

二氮杂苯－水氢键复合物结构性质的理论研究

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摘要 使用密度泛函理论B3LYP方法和从头算MP2方法优化二氮杂苯－水复合物的基态氢键结构和相互作用能的计算。结果表明，邻二氮杂苯－水，间二氮杂苯－水，对二氮杂苯－水复合物具有强的N···H—O氢键相互作用，经基组重叠误差和零点能校正后的氢键相互作用能分别为-20.99, -16.73 和-15.31 kJ/mol，氢键的形成使水的H—O对称伸缩振动频率明显红移（减小）。自然键轨道NBO分析显示，氢键的形成，分子间电荷转移分别为0.0316 e，0.0255 e 和0.0265 e。另外，使用含时密度泛函理论TD-DFT (TD-B3LYP)方法计算了二氮杂苯单体与氢键复合物的第一单重态(n, p^*)激发态的垂直激发能。

关键词 二氮杂苯, 氢键, NBO, 密度泛函理论, MP2

分类号

Theoretical Study on the Structures and Properties of Hydrogen Bonding Complexes between Diazines and Water

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Abstract Density functional theory B3LYP method and second-order Moller-Plesset perturbation theory MP2 method were employed to obtain the optimized geometries of the ground state and interaction energy for diazines and water complexes. The results show that the ground state complexes have strong hydrogen bonding interaction with －20.99, －16.73 and －15.31 kJ/mol after basis set superposition error and zero-point vibration energy correction for pyridazine-water, pyrimidine-water and pyrazine-water, respectively, and large red-shift for the symmetric H—O stretching vibration frequencies due to the formation of N…H—O hydrogen bond in the diazine-water complexes. The NBO analysis indicates that intermolecular charge transfer are 0.0316, 0.0255 and 0.0265 e respectively. In addition, the first singlet (n,π*) vertical excitation energy of the monomer and the hydrogen bonding complexes between diazines and water was investigated by time-dependent density functional theory.

Key words diazine hydrogen bond NBO density functional theory MP2

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