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苯酚-酰胺系列氢键复合物从头计算研究

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摘要 运用G94W量子化学程序包，在HF/6-31G基组水平上对酰胺(DMF,DMA,HCONH2,HCONHCH3andCH3CONH2)与苯酚形成的系列氢键复合物(看作超分子)进行从头计算研究。根据计算结果探讨复合物的稳定性、施体和受体间的电荷转移及几何参数变化等规律。结果表明苯酚与上述一系列酰胺都可形成稳定的氢键复合物，其稳定性次序为CH3CONH2～HCONHCH3＞HCONH2＞DMA＞DMF。结果还表明形成氢键复合物的过程包含着电荷转移，电荷由供体酰胺转移到受体苯酚中，酰胺中C=O键长和苯酚中的O-H键长都明显有规律性地变长。计算结果与实验规律相符。

关键词 苯酚 酰胺 氢键 从头计算法 复合物

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Ab onitio study on the H - bonding complexes formed from phenol and a series of amides

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Abstract The study on hydrogen bonding comlexes (considered as super molecules) formed from phenol and a series of amides was carried out using ab initio calculation at HF/6-31G basis set level (G94W package). The regularities of the stability, the charge transfer between the doner and accepter, and the change of geometric parameters of the complexes were investigated. The results show that some stable complexes can form from phenol and amides (DMF, DMA, HCONH2, HCONHCH3 and CH3CONH2) via hydrogen - bonding. The stability of the complexes is in the order: CH3CONH2 ～HCONHCH3＞HCONH2＞ DMA＞DMF. The calculation results also show that there is an obvious charge transfering in the process of forming the complex, and the charges transfer from the amides to phenil. In addition, the lengths of C=O in the amides and O-H in the phenol are increased obviously. The callculation results are well consistent with the experiments.

Key words PHENOL AMIDES HYDROGEN BONDS AB INITIO CALCULATION COMPLEX

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