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取代基对 1-甲基尿嘧啶与 *N*-甲基乙酰胺氢键复合物中氢键强度的影响

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Effect of Substituents on Hydrogen Bond Strength in Hydrogen-Bonded *N*-methylacetamide and Uracil Complexes

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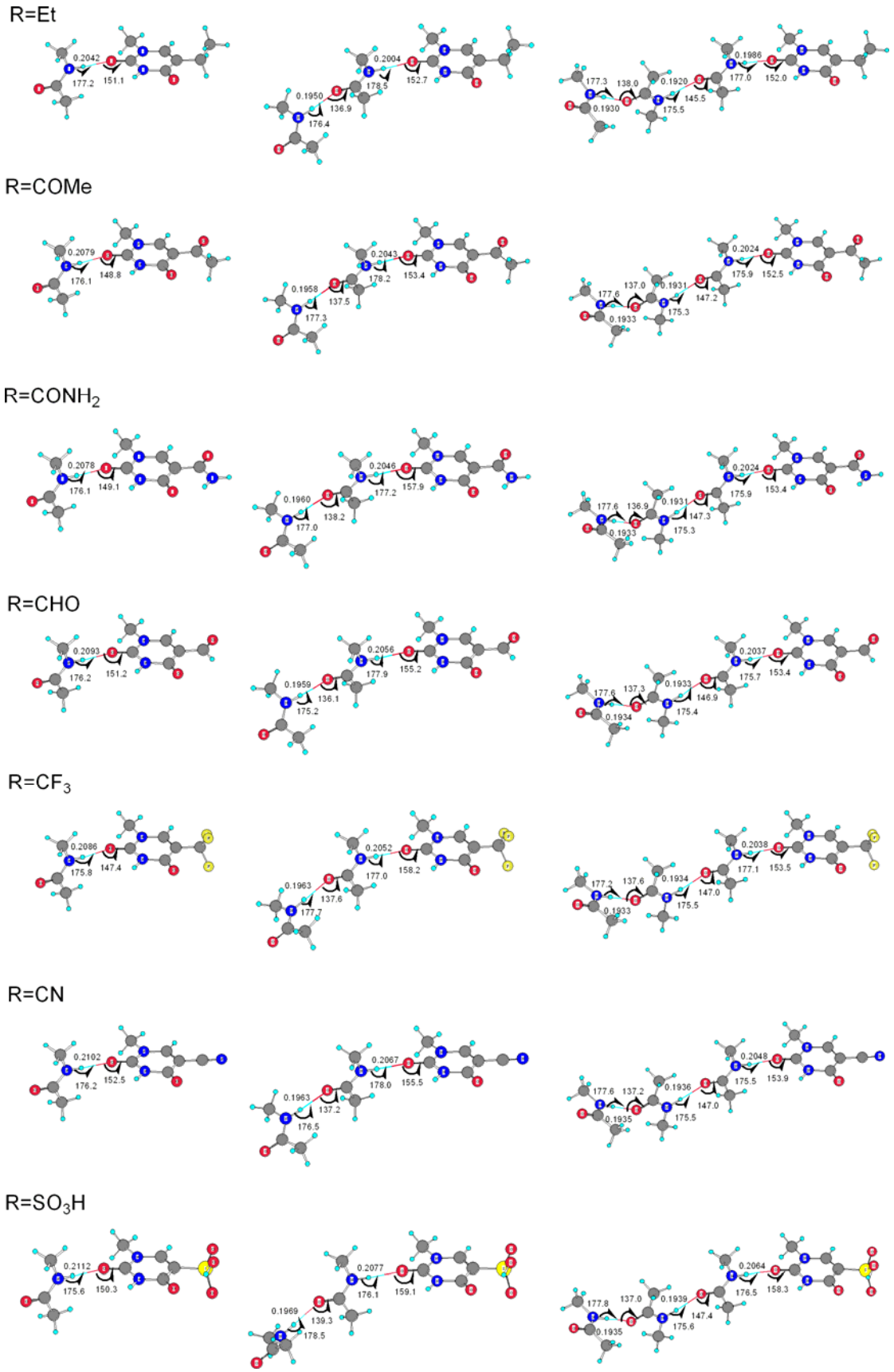

图 S1　21 个氢键复合物的结构

Fig.S1　The optimal geometries of hydrogen-bonded complexes at the B3LYP/6-31+G(*d*, *p*) level

bond length in nm, bond angle in degree