

Quantum chemical study of the hydrogen-bonded HXeOH-H₂O complex.Autorzy

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Streszczenie

A combined MP2 and DFT/B3LYP study of the HXeOH-H₂O complex is presented. These computational methods have been used to extract information on the structural, energetical and vibrational properties of the complex. Additionally, we have applied anharmonic vibrational calculations based on the MP2-computed intermolecular potential energy surface. Large perturbations both on the subunit structures and their fundamental vibrational modes are found upon complexation. Large changes of anharmonicity of the HXeOH subunit reflects the perturbation of the molecule's electronic structure. The computed BSSE-corrected interaction energies are -40.23 and -38.94 kJ mol⁻¹ at the CCSD(T)//MP2 and CCSD(T)//B3LYP levels of theory, respectively. The estimated deformation energy contribution to the interaction energy is about 5%, which is very large compared with classical hydrogen-bonded complexes. The topological analysis of the Electron Localization Function (ELF) was applied to study further the hydrogen-bonded interaction between the two complex partners. The obtained interaction pattern suggests that the interaction between HXeOH and H₂O is a typical hydrogen bond interaction driven mainly by electrostatic interactions.

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