Dihydrogen-bonded complexes of xenon dihydride with water: *Ab initio* calculations and topological analysis of electron localisation function (ELF).

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Streszczenie

b initio calculations on the structures, energetics and vibrational spectra of ternary XeH_2–$(H_2O)_2$ complexes are presented. Three complex structures were found involving dihydrogen bonding between the hydrogens of XeH_2 and water. The lowest energy form is a cyclic structure where the mediating water molecule is bound by a dihydrogen bond to XeH_2 and by a traditional hydrogen bond to the other water molecule. The complex structure is further stabilised by an attraction between the electron lone pairs of the second water molecule and xenon. The calculated interaction energy of this complex is −38.3 kJ mol^{-1} at the CCSD(T)//MP2 level. The two other structures found are about 10–15 kJ mol^{-1} less bound but they still possess relatively strong interactions between complex subunits. The predicted vibrational spectra of these three XeH_2–$(H_2O)_2$ complexes are strongly perturbed compared to the unperturbed monomers, and especially strong shifts are found for the O–H and Xe–H stretching vibrations.

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