THE HF_2^--H_2O COMPLEX: A THEORETICAL STUDY

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In the gas phase, HF_2^- is a hydrogen bonded species with a linear FHF geometry. The F-H distance is short and the hydrogen bond is strong. In the aqueous phase, it is known that the hydrogen bond in HF_2^- is weakened due to hydrogen bonding between HF_2^- and water molecules. We have examined the effect on the hydrogen bond in HF_2^- due to hydrogen bonding between HF_2^- and a single water molecule. For the HF_2^--H_2O complex we have calculated geometries and vibrational frequencies for the equilibrium structure and several transition state structures. We find that the equilibrium structure is a mere 0.2 kcal/mole below the transition state structures indicating that the complex is highly fluctional. We further find that whereas the F-H distance increases for the F atom hydrogen bonded to H_2O, the other F-H distance decreases. The F-F distance is essentially unchanged and the linearity of the FHF geometry is strictly maintained.