



A density functional study of the xenon dihydride-water complex.

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Streszczenie

The $\text{XeH}_2\text{--H}_2\text{O}$ complex has been studied using DFT theory employing various standard basis sets. The complex was found to involve an unconventional dihydrogen bond, i.e. both complex subunits interact via hydrogens ($\text{Xe--H}\cdots\text{H--O}$). The DFT calculations predict an interaction energy of moderate strength (ca. -10 kJ mol^{-1}) and large perturbations of the vibrational spectrum of the complex is noted. Electron localization function analysis has been employed to study the bonding properties of the $\text{XeH}_2\text{--H}_2\text{O}$ complex, and the interaction between XeH_2 and H_2O was found to be mainly of electrostatic origin.

Słowa kluczowe

Dihydrogen bond, Density functional methods, Electron localization function, Xenon dihydrogen, Water complexes

Adres publiczny

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