

On the difference between hydrogen fluoride and hydrogen chloride crystals.

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Streszczenie

The geometrical and energetical parameters of hydrogen fluoride and hydrogen chloride crystals are calculated using the periodic Hartree–Fock method with 6-31G and 6-31G(*d,p*) basis sets. The comparison of the stabilisation energies reveals that HCl crystals are about 75% less stable than HF crystals. The activation energy for collective proton movements are computed and discussed in view of data of isolated infinite chains. The barriers of 13.1 and 40.0 kcal mol⁻¹ at 6-31G(*d,p*) level are found for HF and HCl crystals.

Słowa kluczowe

Ab initio periodic Hartree–Fock method, Hydrogen fluoride crystals, Hydrogen chloride crystals

Adres publiczny

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