Quantum chemical calculations on FXeSiF.

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Streszczenie

Quantum chemical calculations on FXeSiF are reported. The equilibrium structure, energetics, harmonic and anharmonic vibrational frequencies, and an analysis of the nature of bonding, is presented. All calculations are made at the MP2 level, while energetics is also considered via single-point CCSD(T) calculations. Energetical considerations of FXeSiF suggest that it should be stable compared to its decomposition pathways either via its bending coordinate to $Xe+SiF_2$ or via the stretching coordinate to F+Xe+SiF. Analysis of electron localization function (ELF) indicates that both fluorines are bound by interactions of unshared-electron type, i.e. by ionic interactions. The Xe-Si bond, however, is shown to be covalent, and this is the first time a covalent Xe-Si bond is predicted in a neutral molecule.

Adres publiczny

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