

Oxygen-bound fluorine (O-F): *Ab Initio* investigations of the hypofluorous acid dimer.Autorzy

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Streszczenie

Ab initio calculations have been carried out on dimers of hypofluorous acid(HOF)₂. Two stable structures were found, the first one with an almost linear O...H-O hydrogen bridge and F...H-O hydrogen bond and the second one being a cyclic dimer with two F...H-O bonds. The most stable complex determined at the CCSD(T)/6-311++G(2d,2p)//MP2/6-311++G(2d,2p) level is the linear structure, having a stabilization energy of 2.50 kcal/mol. The cyclic structure is only 0.35 kcal/mol higher in energy than the linear one. The organization of the attractors achieved by the topological analysis of the electron localization function (ELF) classifies the interaction in both dimer structures as the unshared-electron type. A transfer of 0.03e between the HOF monomers in the linear structure is deduced from the comparison of the basin populations. The integral density over the F-O attractor basins yields 0.32e for the cyclic structure and 0.27 and 0.37 e for the linear one. The large amount of electron density is concentrated in the regions of the nonbonding valence pairs. The influence, which a dielectric surrounding has on the HOF dimers, has been investigated with the SCRF method, with dielectric constants ranging from 2 to 10 at the B3LYP/6-31G(d,p) level. The cyclic structure which assumed planar (C_{2h}) geometry was found to be unstable (transition state) within a dielectric medium. The calculated frequencies for the linear complex (C₁) agree reasonably well with those observed in a matrix, particularly in the H-O-F deformation region between 1365–1396 cm⁻¹.

Słowa kluczowe

Chemical structure, Electron density, Monomers, Noncovalent interactions, Oligomers

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