Matrix-isolation and computational study of the HXeY…H_2O complexes (Y = Cl, Br, and I).

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Streszczenie

The HXeY···H2O complexes (Y = Cl, Br, and I) are studied theoretically and experimentally. The calculations at the CCSD(T)/def2-TZVPPD level of theory predict two stable structures for Y = Cl and Br and one structure for Y = I, with interaction energies up to about -7 kcal mol(-1). In the experiments, we have identified several infrared absorption bands originating from the H-Xe stretching mode of these complexes in a xenon matrix. The monomer-to-complex frequency shifts of this mode are up to +82 cm(-1) (Y = Cl), +101 cm(-1) (Y = Br), and +138 cm(-1) (Y = I), i.e., the shift is smaller for more strongly bound molecules. Based on the agreement of the experimental and theoretical results, the observed bands are assigned to the most stable planar structure with an O-H···Y-Xe hydrogen bond.

Adres publiczny

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