Experimental and computational study of the HXeI···HY complexes (Y=Br and I).

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Streszczenie

The complexes of HXeI with hydrogen halides HY (Y = Br and I) are studied computationally and experimentally in a xenon matrix. The calculations at the CCSD(T)/def2-TZVPPD level of theory predict several energy minima for the HXeI···HY complexes with interaction energies from −4.69 to −0.23 kcal mol^{-1}. We have identified three bands of the HXeI···HI complexes in the H−Xe stretching region with the monomer-to-complex blue shifts from +37 to +96 cm^{-1}, and three bands of the HXeI···HBr complexes with blue shifts from +88 to +157 cm^{-1}. The structural assignments are done on the basis of the strong H−Xe and HY stretching bands and the decomposition rates upon broadband IR irradiation. The experimental bands with larger shifts are assigned to the most stable structures of the HXeI···HY complexes with the Y−H···I hydrogen bond.I.

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