

Intra- and intermolecular hydrogen bonding in formohydroxamic acid complexes with water and ammonia: infrared matrix isolation and theoretical study.

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Streszczenie

The complexes of formohydroxamic acid with water and ammonia have been studied using FTIR matrix isolation spectroscopy and MP2 calculations with a 6-311++G(2d,2p) basis set. The analysis of the experimental spectra of the HCONHOH/H₂O(NH₃)/Ar matrixes indicates formation of strongly hydrogen-bonded complexes in which the NH group of formohydroxamic acid acts as a proton donor toward the oxygen atom of water or the nitrogen atom of ammonia. The NH stretching vibration of formohydroxamic acid exhibits 150 cm⁻¹ red shift in the complex with water and 443 cm⁻¹ red shift in the complex with ammonia as compared to the NH stretch of the HCONHOH monomer. The theoretical calculations indicate stability of five isomers for the water complex and three isomers for the ammonia complex. The most stable are the cyclic structures in which the water or ammonia molecules are inserted within the intramolecular hydrogen bond of the formohydroxamic acid molecule and act as proton donors for the CO group and proton acceptors for the OH group of the formohydroxamic acid molecule. In spite of their stability the cyclic structures have not been observed in the matrixes which indicates high energy barrier for their formation, the reaction of complex formation is under kinetic and not thermodynamic control.

Adres publiczny

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