The interaction of formohydroxamic acid with carbon monoxide: FTIR matrix isolation and quantum chemistry studies.

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Streszczenie

Argon matrix infrared spectra of the complexes formed between formohydroxamic acid (HCONHOH) and carbon monoxide have been recorded. The experimental results indicate formation of three isomeric complexes. In two complexes the NH or OH groups of formohydroxamic acid are attached to the carbon atom of the CO molecule and in the third complex the NH group interacts with the oxygen atom of CO. The formohydroxamic acid complex with two CO molecules is also trapped in the matrix. One of the two CO molecules interacts with the NH group and the second one with the OH group of HCONHOH, in both cases the site of interaction is the carbon atom of CO. Theoretical studies of the structure and spectral characteristics of the complexes were carried out on the DFT(B3LYP)/6-311++G(2d,2p) level. The calculated vibrational frequencies for the complexes present in the matrices are in good agreement with the experimental data. The calculations show also an additional potential energy minimum corresponding to the complex in which the OH group of formohydroxamic acid is attached to the oxygen atom of carbon monoxide.

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