

The interaction of formohydroxamic acid with nitrogen: FTIR matrix isolation and ab initio studies.

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Streszczenie

Argon matrix infrared spectra of the complexes formed between formohydroxamic acid, HCONHOH (FHA) and nitrogen have been recorded. The experimental results indicate formation of two isomeric complexes in which the nitrogen atom of the N₂ molecule is attached to the NH or OH groups of FHA. Theoretical studies of the structure and spectral characteristics of the complexes were carried out on the MP2 level with the 6-311++G(2d,2p) basis set. The calculated vibrational frequencies for the complexes present in the matrices are in good agreement with the experimental data.

Słowa kluczowe

Formohydroxamic acid, Nitrogen, Hydrogen bond, Molecular complexes, Matrix isolation, Infrared spectra

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