

## Infrared matrix isolation studies and ab initio calculations of formhydroxamic acid.

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The infrared absorption spectra of formhydroxamic acid (HCONHOH) and its isotopic analogues (HCONDOD, HCO<sup>15</sup>NHOH) isolated in argon and nitrogen matrices have been recorded for the first time. The infrared spectra prove that this molecule exists as the keto tautomer with an intramolecular hydrogen bond in solid argon and nitrogen. The normal coordinate analysis indicated strong coupling between amide grouping vibrations. Theoretical studies of the structure and spectral characteristic of the formhydroxamic acid molecule, carried out on both MP2 and B3LYP levels with the 6-311++G(2d,2p) basis set, were in accordance with the experimental data.

Słowa kluczowe

Amides, Molecules, Oscillation, Nitrogen, noncovalent interactions

Adres publiczny<https://doi.org/10.1021/jp013643p>Strona internetowa wydawcy<https://www.acs.org/content/acs/en.html>