



Matrix infrared spectra and ab initio calculations of the nitrous acid complexes with nitrogen monoxide.

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Streszczenie

Complexes between trans and cis isomers of nitrous acid and nitrogen monoxide have been isolated in argon matrices and studied using FTIR spectroscopy and ab initio calculations at the ROMP2 level. The calculations indicate formation of four hydrogen-bonded complexes with *trans*- or *cis*-HONO isomer bound to nitrogen or oxygen atoms of NO molecule. Comparison of the calculated frequencies with the frequencies of the complexes trapped in solid argon proved that the more stable ON...HONO trans and ON...HONO cis complexes with an acid molecule attached to nitrogen atom are trapped in the matrix.

Słowa kluczowe

Molecular structure, Molecules, Monomers, Nitrogen, Oscillation

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<https://www.acs.org/content/acs/en.html>