Matrix isolation and DFT studies of nitrous acid complexes with nitrogen dioxide.

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Streszczenie

Complexes between *trans* or *cis* isomers of nitrous acid and nitrogen dioxide have been isolated in argon matrices and studied using Fourier transform infrared (FTIR) spectroscopy and density functional theory (DFT) calculation at B3LYP level with the 6-311++G(2d,2p) basis set. Six perturbed vibrations of *trans*-HONO and three perturbed vibrations of*cis*-HONO isomers were identified for the *trans* and *cis*-HONO complexes, respectively. The perturbed asymmetric stretching vibration of NO_2 molecule was also identified for the two complexes. The experimental spectra suggest and the theoretical calculations confirm that there is double interaction in the two complexes. The OH group of HONO molecule serves as a proton donor to an oxygen atom of NO_2, and in addition to hydrogen bonding there is an electrostatic attraction between an oxygen atom of OH and nitrogen atom of NO_2 molecules. Calculated counterpoise corrected interaction energy is equal to −1.19 and −1.10 kcal/mol for NO_2…*cis*-HONO and NO_2…*trans*-HONO complexes, respectively.

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