Ab initio calculations and matrix infrared spectra ot the nitrous acid complexes with HF and HCl.

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Streszczenie

Theoretical studies of the structure and spectral characteristics of the complexes formed by *trans*- and *cis*-HONO isomers with hydrogen fluoride and hydrogen chloride were carried out on the electron correlation level with the 6-311++G(2d,2p) basis set. The calculations demonstrate formation of three stable complexes between *trans*-HONO isomer and HX and five stable complexes between *cis*-HONO isomer and HX. In the most stable HX···*trans*-HONO, HX···*cis*-HONO complexes the HX subunit acts as a proton donor and interacts with an oxygen atom of the OH group which is a proton acceptor. The complexes predicted to be the most stable ones were identified and characterized in argon matrices. Six and five perturbed HONO vibrations of *trans*-HONO isomer were identified, respectively, for HF···*trans*-HONO and HCl···*trans*-HONO complexes whereas two perturbed vibrations of *cis*-HONO isomer were identified for HF···*cis*-HONO and HCl···*cis*-HONO complexes.

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