Infrared matrix isolation and theoretical studies of SO_2-HNO_3 and SO_2-HONO systems.

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Streszczenie

Argon matrix infrared spectra of sulphur dioxide complexes with nitric or nitrous acid indicate formation of hydrogen-bonded structures. The red shifts of the OH stretching modes are equal to ca. 179, 51 and 40 cm^{-1} in SO_2–HNO_3, SO_2–HONO-trans and SO_2–HONO-cis complexes, respectively. Theoretical studies of the structure and spectral characteristics of the title complexes were carried out on the electron correlation level with 6-31G(d) basis set. For all studied systems only one stable structure was found with the OH group interacting with one oxygen atom of the sulphur dioxide molecule. The calculated infrared spectra reproduce well the frequencies and the intensities of the measured spectra.

Adres publiczny

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