

Hydrogen bonding in allene complexes with nitric and nitrous acids: theoretical and infrared matrix isolation study.

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Streszczenie

The complexes formed by HNO_3 and the *trans*-HONO isomer with allene in argon matrixes have been identified and characterized by help of FTIR spectroscopy. The experimental spectra proved the formation of two types of complexes with slightly different structures for the two studied systems. The theoretical studies of the structure and spectral characteristics of the complexes formed between HNO_3 , *trans*-HONO, *cis*-HONO, and the allene molecule were carried out at the MP2 and DFT(B3LYP) levels of theory with the 6-311++G(2d,2p) basis set. In agreement with experimental data the calculations resulted in two stationary points (A and B) for each of the three studied systems. All complexes (A and B) are stabilized by the O-H... π bond; however, in the A complexes there exists also a weak C-H...O or C-H...N interaction. The topological analysis of the distribution of the charge density (AIM theory) confirmed the existence of a double interaction in the A complexes. According to the eight AIM-based criteria for hydrogen bonding the C-H...O, C-H...N interactions are of hydrogen-bonded nature.

Słowa kluczowe

Interaction energies, Chemical structure, Allenes, Molecules, Oscillation

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