

Matrix isolation FTIR and theoretical study of weakly bound complexes of isocyanic acid with nitrogen.

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Streszczenie

Weak complexes of isocyanic acid (HNCO) with nitrogen were studied computationally employing MP2, B2PLYPD3 and B3LYPD3 methods and experimentally by FTIR matrix isolation technique. The results show that HNCO interacts specifically with N₂. For the 1:1 stoichiometry, three stable minima were located on the potential energy surface. The most stable of them involves a weak, almost linear hydrogen bond from the NH group of the acid molecule to nitrogen molecule lone pair. Two other structures are bound by van der Waals interactions of N...N and C...N types. The 1:2 and 2:1 HNCO complexes with nitrogen were computationally tracked as well. Similar types of interactions as in the 1:1 complexes were found in the case of the higher stoichiometry complexes. Analysis of the HNCO/N₂/Ar spectra after deposition indicates that the 1:1 hydrogen-bonded complex is prevalent in argon matrices with a small amount of the van der Waals structures also present. Upon annealing, complexes of the 1:2 and 2:1 stoichiometry were detected as well.

Słowa kluczowe

hydrogen bond, van der Waals interaction, vibrational spectroscopy, computational chemistry, molecular complex, atmospheric chemistry, HNCO

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