



Dimerization of the keto tautomer of acetohydroxamic acid-infrared matrix isolation and theoretical study.

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Streszczenie

Dimerization of the keto tautomer of acetohydroxamic acid has been studied using FTIR matrix isolation spectroscopy and DFT(B3LYP)/6-31+G(d,p) calculations. Analysis of CH₃CONHOH/Ar matrix spectra indicates formation of two dimers in which two intramolecular CO...HON bonds within two interacting acetohydroxamic acid molecules are retained. A chain dimer I is stabilized by the intermolecular CO...HN hydrogen bond, whereas the cyclic dimer II is stabilized by two intermolecular NH...O(H)N bonds. Twelve vibrations were identified for dimer I and six vibrations for dimer II; the observed frequency shifts show a good agreement with the calculated ones for the structures I and II. Both dimers have comparable binding energies ($= -7.02, -6.34 \text{ kcal mol}^{-1}$) being less stable than calculated structures III and IV ($= -9.50, -8.87 \text{ kcal mol}^{-1}$) in which one or two intramolecular hydrogen bonds are disrupted. In the most stable 10-membered cyclic dimer III, two intermolecular CO...HON hydrogen bonds are formed at expense of intramolecular hydrogen bonds of the same type. The formation of the less stable (AHA)₂ dimers in the studied matrixes indicates that the formation of (AHA)₂ is kinetically and not thermodynamically controlled.

Słowa kluczowe

Acetohydroxamic acid, Molecular aggregates, Hydrogen bonding, Infrared spectroscopy, Matrix isolation, Computational methods

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