



Formaldoxime hydrogen bonded complexes with ammonia and hydrogen chloride.

Autorzy

Barbara Golec

Małgorzata Mucha

Magdalena Sałdyka

Austin J. Barnes

Zofia Mielke

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Streszczenie

An infrared spectroscopic and MP2/6–311++G(2d,2p) study of hydrogen bonded complexes of formaldoxime with ammonia and hydrogen chloride trapped in solid argon matrices is reported. Both 1:1 and 1:2 complexes between formaldoxime and ammonia, hydrogen chloride have been identified in the CH₂NOH/NH₃/Ar, CH₂NOH/HCl/Ar matrices, respectively, their structures were determined by comparison of the spectra with the results of calculations. In the 1:1 complexes present in the argon matrices the OH group of formaldoxime acts as a proton donor for ammonia and the nitrogen atom acts as a proton acceptor for hydrogen chloride. In the 1:2 complexes ammonia or hydrogen chloride dimers interact both with the OH group and the nitrogen atom of CH₂NOH to form seven membered cyclic structures stabilized by three hydrogen bonds. The theoretical spectra generally agree well with the experimental ones, but they seriously underestimate the shift of the OH stretch for the 1:1 CH₂NOH...NH₃ complex

Słowa kluczowe

Formaldoxime, Ammonia, Hydrogen bond, Matrix isolation, Ab initio calculations, molecular complexes

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