

THE FORMAMIDE₂-H₂O COMPLEX: STRUCTURE AND HYDROGEN BOND COOPERATIVE EFFECTS

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The adduct formamide₂-H₂O has been detected in a supersonic expansion and its rotational spectra in the 5-13 GHz frequency region characterized by narrow-band molecular beam Fourier transform microwave spectroscopy (MB-FTMW). The spectrum shows the hyperfine structure due to the presence of two ¹⁴N-nuclei. This hyperfine structure has been analyzed and the determined quadrupole coupling constants together with the rotational constants have been a key for the identification of the adduct structure on the light of ab initio computations. The rotational parameters are consistent with the formation of a three body cycle thanks to the double proton acceptor/proton donor character of both formamide and water. The low value of the planar moment of inertia P_{cc} indicates that the heavy atom skeleton of the cluster is essentially planar. A detailed analysis of the results reveals the subtle effects of hydrogen bond cooperative effects in this system.