

A STUDY OF THE FORMAMIDE-(H₂O)₃ COMPLEX BY MICROWAVE SPECTROSCOPY

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The adduct formamide-(H₂O)₃ has been detected in a supersonic expansion and its rotational spectrum characterized in the 5-13 GHz frequency region by narrow-band molecular beam Fourier transform microwave spectroscopy (MB-FTMW). The spectrum shows the hyperfine structure due to the presence of one ¹⁴N-nuclei and small splittings due to a tunnelling motion of the complex. The spectra has been analyzed using a two-state Hamiltonian including Coriolis coupling terms to determine the vibrational spacing. 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 four body cycle thanks to the double proton acceptor/proton donor character of both formamide and water. The rotational data are consistent with a non-planar heavy atom skeleton.