

A ROTATIONAL STUDY OF THE METHYL CARBAMATE-(H₂O)_n n=1,2 COMPLEXES: MICROWAVE SPECTRUM, INTERNAL ROTATION AND HYPERFINE STRUCTURE.

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The rotational spectrum of methyl carbamate has been recorded in the 2-8 GHz frequency region using a chirped-pulse Fourier transform microwave spectrometer. The carrier gas was seeded with water and methyl carbamate vapors for the formation of microsolvated complexes. Complexes with one and two molecules of water have been detected. Both spectra show the fine structure arising from the internal rotation of the methyl top together with the hyperfine structure due to the presence of one ¹⁴N nucleus. The spectra were further registered in the 5-18 GHz frequency region by the higher resolution supersonic expansion cavity Fourier transform microwave spectroscopy to analyze more accurately the hyperfine structure. The determined rotational parameters provide the key for the identification of the complexes in the light of ab initio computations. Both the methyl group internal rotation barrier and the quadrupole coupling constants show interesting trends in going from isolation to the microsolvated complexes.