FOURIER TRANSFORM MICROWAVE SPECTRA OF N-METHYLFORMAMIDE

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In order to understand the dynamical behavior of the peptide bond in “peptide molecules: X-CONH-Y”, we have chosen N-methylformamide (N-MFA) as a simplest system with X = H and Y = CH₃. The microwave spectrum of the most stable trans form of N-MFA was studied by Fantoni and Caminati, a who assigned and analyzed only the A state of the CH₃ internal rotation and thus reported an estimated potential barrier $V_3$. Kitano and Kuchitsu b determined the molecular structure of trans N-MFA by using electron diffraction, but they could not detect the higher energy cis conformer. We report here the rotational spectrum of both the trans and cis forms of N-MFA using FTMW spectrometers at NIST and KAIT, in the frequency region from 5 to 36 GHz, with either Ne or Ar as a buffer gas in a reservoir nozzle maintained at about 50°C. We confirmed the assignment of Ref.a for the trans A state and extended the observation to low-J transitions. The spectra of four trans isotopomers $^{13}$C, $^{15}$N, and $^{18}$O were observed to derive an $r_s$ structure, which is in good agreement with the electron diffraction and ab initio results. The $V_3$ value of trans is approximately 60 cm$^{-1}$, which is 4.5 times smaller than the value of cis form which was determined to be 279 cm$^{-1}$.

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