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 = $CH_3$. 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 $CH_3$ 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$^o$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$^{-1}$.

[a] A. C. Fantoni and W. Caminati *J. Chem. Soc. Faraday Trans.* **92**, 342 (1995).
[b] M, Kitano and K. Kuchitsu *Bull. Chem. Soc. Jpn.* **47**, 631 (1974).