N-tert-butylformamide－methanol 錯体の フーリエ変換マイクロ波分光

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Fourier transform microwave spectroscpy of *N-tert*-butylformamide　methanol complex

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The pure rotational spectra of *N-tert*-butylformamide　methanol complex have been investigated with a pulsed beam Fourier transform microwave spectrometer. Two isomers of the C=O···$HOCH_3$ type hydrogen bonding complex were observed, the spectra of both isomers exhibit the A – E splitting due to internal rotation of the methyl group of methanol and the ^{14}N nuclear quadorupole hyperfine structure. The spectrum was analyzed to determine rotational constants, Coriolis-like coupling parameters which characterize interaction between the internal rotation and the overall rotation, and the nuclear quadrupole coupling constants. The barrier height to the methyl group internal rotation was estimated from the Coriolis-like coupling parameters and the effective rotational constants for the A and E symmetry states. Structures of the complexes were derived from the rotational constants and those of the *N-tert*-butylformamide and methanol monomers.

X – CONH　Y

N-tert-butylformamide　$HCONHC(CH_3)_3$　NtBF

$NtBF\cdots H_2O$　$NtBF\cdots(H_2O)_2$

$NtBF\cdots CH_3OH$

1

2

0.8 mm

NtBF

80

3.5

1

1000

NtBF

9.3　11.5 GHz

1

1043　1046 MHz

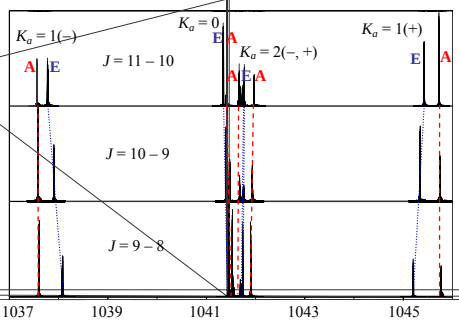


図 1. isomer-1a の回転構造パターン

κ = -0.995 *a*-type *R* branch J = 9 – 8, 10 – 9, 11 – 10, K_a = 0, 1, 2 *b*-type *c*-type A–E N NtBF···CH_3OH isomer-1a isomer-1a isomer-1a A–E isomer-1b κ = -0.868 isomer-1b *a*-type *b*-type

Hougen [3]

N-methylaniline [2] *N*,*N*-dimethylacetamide [4]

$$H = h_V + AJ_z^2 + BJ_x^2 + CJ_y^2 + (Centrifugal\ distorsion\ terms : Watoson's - A) + iqJ_z + isJ_x + itJ_y + (higher - order\ Coriolis\ terms) + H_{eQq} \quad (1)$$

NtBF···CH_3OH 1a 1b 1

2

NtBF···CH_3OH *ab initio* C=O···$HOCH_3$ isomer *ab initio* 1a 1b

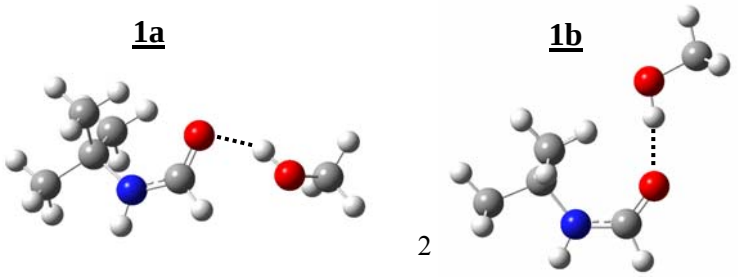
1 NtBF···CH_3OH (MHz)[a]

	Isomer-1a	Isomer-1b
A_1	3757.0(23)	2313.2022(24)
B_1	524.9312(17)	786.70371(28)
C_1	516.8049(16)	678.44805(19)
A_2	3.36(56)	0.75134(91)
B_2	0.010610(99)	0.005282(36)
C_2	0.005917(98)	0.002865(27)
q_2	53.351(30)	50.6557(16)
s_2	4.991(21)	4.205(22)
χ_{aa}	0.661(94)	1.648(33)
χ_{bb}-χ_{cc}	5.29(22)	5.489(15)

[a]

q_2, s_2 A_1 A_2

1a **1b**



2

V_3 1a, 1b 220 cm^{-1} 200 cm^{-1}

V_3 373.1 cm^{-1}

2 NtBF···CH_3OH

1) 2006 4P092.
2) M. Fujitake, J. Aoyama, N. Ohashi, *J. Mol. Spectrosc.* **235** (2006) 27 – 34.
3) J. T. Hougen, *J. Mol. Spectrosc.* **89** (1981) 296 – 327.
4) M. Fujitake, Y. Kubota, N. Ohashi, *J. Mol. Spectrosc.* **236** (2006) 97 – 109.