N-tert-butylformamide-$(H_2O)_n$ complexes (n=1,2)

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Fourier transform microwave spectroscopy of N-tert-butylformamide-$(H_2O)_n$ complexes (n=1,2)

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Abstract

The jet-cooled Fourier transform microwave spectra of N-tert-butylformamide-$(H_2O)_n$ complexes (n=1,2), two isomers of N-tert-butylformamide-H_2O and one of N-tert-butylformamide-$(H_2O)_2$, were recorded in region of 9-17 GHz, and were analyzed to determine rotational constants, distortion constants and nuclear quadrupole coupling constants. From these constants, we determined molecular structures of these complexes in order to study effects on N-tert-butylformamide from water.

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N-tert-butylformamide (NTBF)

NTBF Z-form E-form

Z-form 1 2

NTBF

90 H_2O 1% Ne 3.0atm

ab initio (MP2/6-31G) 10~13GHz

0.5MHz 300 NTBF

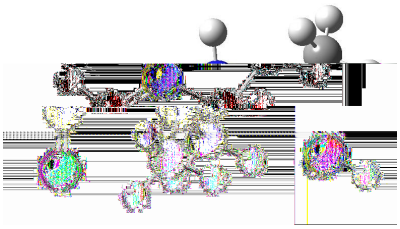
1000 10000 9~17GHz

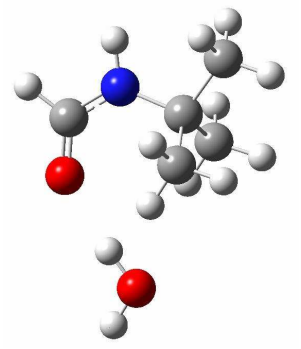
3 NTBF-H_2O-isomer1, NTBF-H_2O-isomer2, NTBF-$(H_2O)_2$ (Fig. 1) a-type R-branch 28,28,38 b-type R-branch 10,13,9

$\Delta F = \Delta J$ 3

Table

NTBF





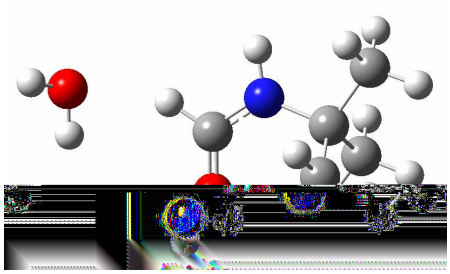


Fig. 1 NTBF-H_2O-isomer 1 NTBF-H_2O-isomer 2 NTBF-$(H_2O)_2$

NTBF-H_2O

ab initio isomer 1 NTBF

(Fig. 2) NTBF

isomer 1 0.67u ^{2}

μ_c

c-type

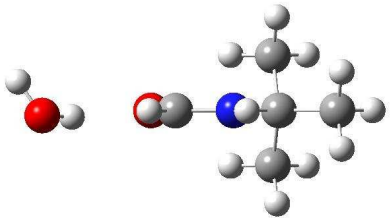


Fig. 2 NTBF-H_2O-isomer 1

NTBF isomer 2 0.32u ^{2} isomer 2 NTBF

χ_{cc} NTBF 5%

isomer 1

NTBF-$(H_2O)_2$

NTBF CHO

NTBF-$(H_2O)_2$

NTBF-H_2O-isomer1, NTBF-H_2O-isomer2, NTBF-$(H_2O)_2$

Table

Molecular constants (in MHz) of N-tert-butylformamide-$(H_2O)_n$ complexes (n=1,2) in the ground vibrational state

	NTBF-H_2O		NTBF-$(H_2O)_2$
	isomer 1	isomer 2	
A	4035.3206(15)	2408.17758(47)	2464.81978(19)
B	814.70860(80)	1274.19884(16)	582.657585(85)
C	798.42334(79)	1022.51230(12)	526.943517(68)
χ_{aa}	1.7486(61)	1.6674(48)	1.7760(73)
$\chi_{bb} - \chi_{cc}$	5.5010(43)	5.4849(65)	5.3409(49)