SEP分光法によるC_3Nラジカルの$\tilde{A}$状態の観測 (3)

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Observation of the $\tilde{A}$ state of the C_3N radical by SEP spectroscopy 3

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Four $^2\Sigma^+$ and eight $^2\Pi$ vibronic bands in the $\tilde{A}\,^2\Pi_i$ state of C_3N have been observed by stimulated emission pumping (SEP) spectroscopy. The energy level structure and small splittings of the spin components in the $^2\Pi$ vibronic bands show that the observed bands correspond to K_a = 0 and 1 levels of an asymmetric top. This means the $\tilde{A}$ state has a bent molecular structure due to a large Renner-Teller effect. For each vibrational state, rotational constants and spin-rotation constants were determined by the least-squares analysis using an asymmetric top Hamiltonian.

【序】　C_3N　2

$\tilde{X}\,^2\Sigma^+$ [1,2,3], $\tilde{B}\,^2\Pi_i$ [4]

C_3N

$\tilde{A}\,^2\Pi_i$　*ab initio*

[5]　C_3N　C_4H

C_3N　$\tilde{A}$　SEP

[6]　C_3N

$\tilde{A}$

【実験】　$\tilde{B}$　SEP

Ar　0.3　C_3N

2

$\tilde{B}$　v_3 = 1 ($^2\Pi$, 28800 cm^{-1})　v_3 = v_4 = 1 ($^2\Sigma^+$, 29144 cm^{-1})

SEP

【結果と考察】　1　SEP

2(a)　$^2\Pi_i$

Renner-Teller

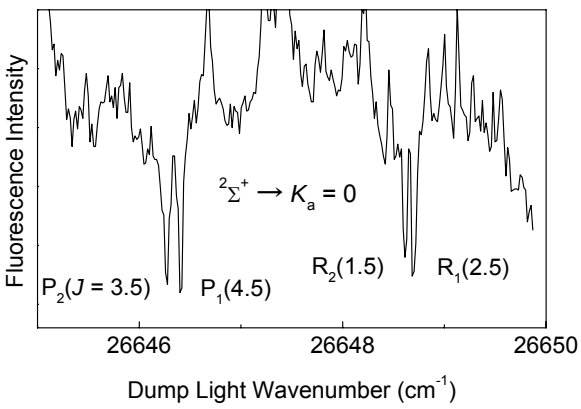

図 1　観測した SEP スペクトル

2(b)

4 $^2\Sigma \rightarrow ^2\Sigma$

8 $^2\Pi_P \rightarrow ^2\Pi_P$ (P = 1/2, 3/2)

$\tilde{A}$

$^2\Pi$

2.6 ~ 8.4 cm^{-1}

$\tilde{B}$

1

$\tilde{A}$ Renner-Teller

図 2 RT 効果の大きさによる準位のエネルギー変化

K_a = 0, 1

K_a = 0, 1

B–C *ab initio* *A*

C_3N $\tilde{A}$ $\tilde{X}$, $\tilde{B}$

$\tilde{A}$

(in cm^{-1})

T_v	ΔE	A	$(B+C)/2$ [a]	ε_{aa}	ε_{bb}	σ
1790.038(3)	0	51.394(2)	0.16467(7)	-2.190(3)	0 [b]	0.007
2030.937(5)	241	52.537(3)	0.16492(8)	-6.089(3)	0 [b]	0.007
2288.774(4)	499	25.743(3)	0.1663(1)	-2.686(4)	0 [b]	0.009
2496.468(4)	706	31.15(1)	0.1648(2)	-8.11(1)	-0.067(4)	0.018

[a] Value of *B–C* is fixed to 16 MHz calculated by an *ab initio* method.

[b] Fixed.

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