1,4-

Analysis of the electronic spectra of jet-cooled 1,4-bis(phenylethenyl)benzene

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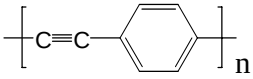
The S_1-S_0 electronic spectra of jet-cooled 1,4-bis(phenylethynyl)benzene were observed by means of the fluorescence excitation and the single-vibronic-level dispersed fluorescence methods. The 0-0 transition was measured at 31 270 cm^{-1}. 7 S_0-state vibrations and 2 S_1-state ones were assigned to respective normal vibrations. Two series of progressions with frequency intervals of 72 cm^{-1} and 128 cm^{-1} appeared on the excitation spectrum. There are two candidates of the assignment of which are in-plane and out-of plane bending vibrations or in-phase and out-of-phase torsional vibrations.

1,4- 1 a

(a) 1,4-Bis(phenylethynyl)benzene



π

π (b) Poly-phenylethynyl compound

図１　研究対象分子

π

π

202 cm^{-1}

8 20

1,4- 2005 4 2006 2

J. Phys. Chem. A Stuart J. Greaves Cavity Ring-Down

(SVL)

9.7×10^{-8} Torr

Cavity Ring-Down

220

1,4-

220 He Down stream

Nalumi-750 50 μm 23 cm^{-1} FWHM

B3LYP/6-311Gd

Herzberg

S_0 ππ*

S_1 0-0 31270 cm^{-1}

7 K 24 K

0^0 SVL

SVL

1132 cm^{-1}

$12_1(a_g)$

160 cm^{-1} $18_1(a_g)$

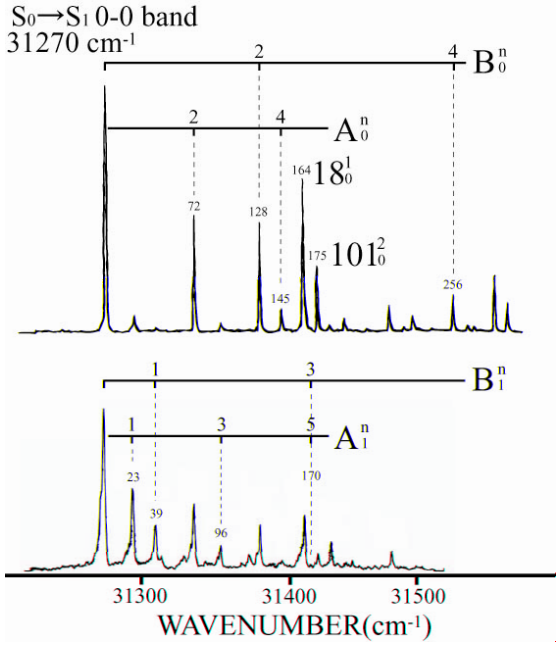


図２　ジェット中の蛍光励起スペクトル

18 S_1 164 cm^{-1}

A^n_0

B^n_0

SVL

A^n_1 B^n_1

S_0 12 cm^{-1} 22 cm^{-1}

A^n_2 B^n_2

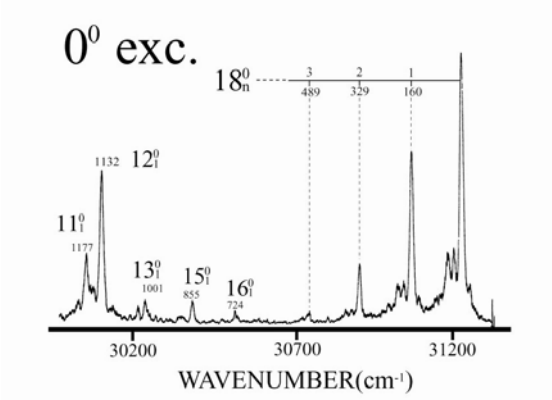


図３　SVL 蛍光分光スペクトル

ππ*

A B

SVL S_0

表　構造最適化計算から得られた低振動数の振動

振動型	番号（表現）	振動数[(a)]
Out-of-phase ねじれ運動	29 (b_{1g})	31 cm^{-1}
In phase ねじれ運動	24 (a_u)	21 cm^{-1}
面内変角振動	74 (b_{2u})	21 cm^{-1}
面外変角振動	102 (b_{3u})	17 cm^{-1}

(a)0.9613 で Scaled された振動数