

## 266 nm 激光光解 C<sub>2</sub>H<sub>5</sub>SSC<sub>2</sub>H<sub>5</sub> 产物的激光诱导荧光光谱

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## Laser-Induced Fluorescence Spectra of the Photolyzed Products of C<sub>2</sub>H<sub>5</sub>SSC<sub>2</sub>H<sub>5</sub> by 266 nm Laser

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表 S1 激发态  $\tilde{B}$  态振动频率计算结果

Table S1 Vibrational frequencies of the  $\tilde{B}$  state of ethylthio radical

Vibration mode	Symmetry	CAS <sup>a</sup> /cm <sup>-1</sup>	CIS <sup>b</sup> /cm <sup>-1</sup>
$E_{\tilde{B}-\tilde{X}}$	$\nu_{00}^{\tilde{B}-\tilde{X}}$	23695	26374
C-C-S bend	$\nu_{11}$ A'	266	322
CH <sub>3</sub> rotation	$\nu_{18}$ A''	314	280
C-S stretch	$\nu_{10}$ A'	424	663
CH <sub>3</sub> wag (out)	$\nu_{17}$ A''	864	780
CH <sub>2</sub> rock	$\nu_{16}$ A''	983	907
CH <sub>2</sub> +CH <sub>3</sub> wag (in)	$\nu_9$ A'	1004	961
C-C stretch	$\nu_8$ A'	1144	1163
CH <sub>2</sub> wag (in)	$\nu_7$ A'	1278	1363
CH <sub>2</sub> +CH <sub>3</sub> rock	$\nu_{15}$ A''	1334	1330
CH <sub>3</sub> umbrella (in)	$\nu_6$ A'	1517	1508
C-H <sub>3</sub> rock	$\nu_{14}$ A''	1562	1548
C-H <sub>2</sub> +CH-H <sub>2</sub> sissors (in)	$\nu_5$ A'	1597	1601
H-CH-H scissors (in)	$\nu_4$ A'	1617	1620
CH <sub>3</sub> umbrella stretch (in)	$\nu_3$ A'	3137	3105
C-H <sub>3</sub> stretch (in)	$\nu_2$ A'	3256	3257
C-H <sub>2</sub> stretch (in)	$\nu_1$ A'	3297	3324
C-H <sub>3</sub> stretch (out)	$\nu_{13}$ A''	3306	3312
C-H <sub>2</sub> stretch (out)	$\nu_{12}$ A''	3413	3416

calculated <sup>a</sup> at the CASSCF/6-311++G(*d,p*) level, <sup>b</sup> at the CIS/6-311++G(*d,p*) level.

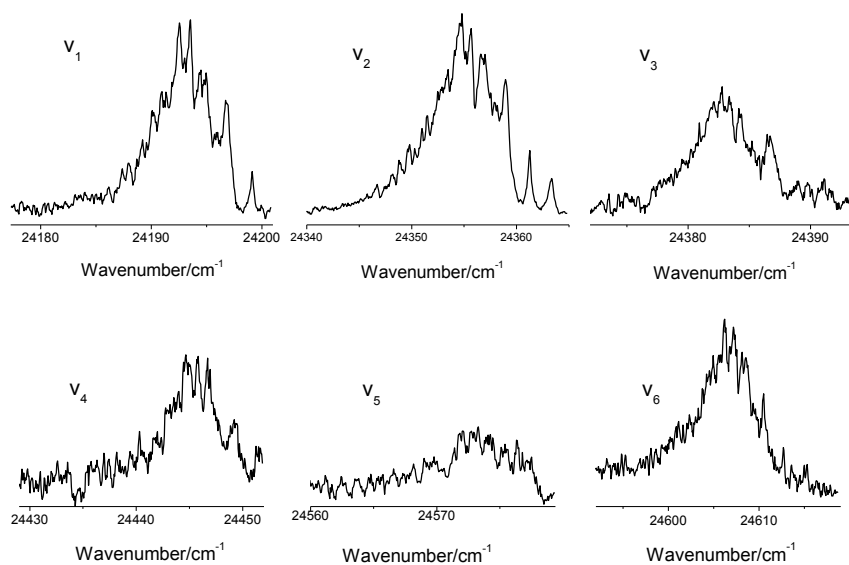


图 S1  $\nu_1$ - $\nu_6$  轮廓图

Fig.S1 Contour of the  $\nu_1$ - $\nu_6$