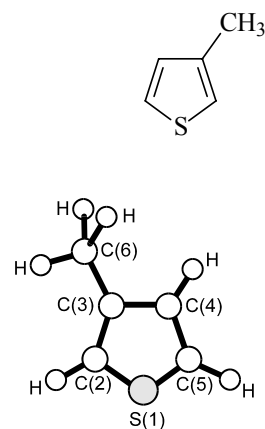


**638 C<sub>5</sub>H<sub>6</sub>S**ED, MW, *ab initio*  
calculations**3-Methylthiophene****C<sub>s</sub>** (main conformer)

$r_g$	Å <sup>a)</sup>	$\theta_\alpha$	deg <sup>a)</sup>
C(2)–H	1.101(5) <sup>b)</sup>	C(2)–S–C(5)	91.6(2)
C(4)–H	1.104(5) <sup>b)</sup>	S–C(2)=C(3)	113.3(5)
C(5)–H	1.102(5) <sup>b)</sup>	S–C(5)=C(4)	111.3(3)
C(6)–H	1.117(5) <sup>b)</sup>	C(2)=C(3)–C(4)	110.1 <sup>c)</sup>
C(3)–C(6)	1.497(6)	C(3)–C(4)=C(5)	113.8 <sup>c)</sup>
C(3)–C(4)	1.441 <sup>c)</sup>	C(2)=C(3)–C(6)	123.2(11)
S–C(2)	1.719(2) <sup>d)</sup>	S–C(2)–H	121.0 <sup>c)</sup>
S–C(5)	1.717(2) <sup>d)</sup>	C(5)=C(4)–H	123.9 <sup>c)</sup>
C(2)=C(3)	1.370(3) <sup>d)</sup>	S–C(5)–H	121.0 <sup>c)</sup>
C(4)=C(5)	1.368(3) <sup>d)</sup>	C(3)–C(6)–H	112(2)



The molecule, except for the methyl hydrogen atoms, was assumed to be planar. Local C<sub>3v</sub> symmetry and no tilt were assumed for the methyl group. The torsional vibration of the methyl group was treated as a large-amplitude motion. One C–H bond of the methyl group in the most stable conformer is eclipsed with respect to the C(2)=C(3) bond ( $\angle \text{H–C(6)–C(3)=C(2)} = 0^\circ$ , see figure). According to the results of HF/3-21G\* calculations, the second conformer with  $\tau = 90^\circ$  (C<sub>1</sub> symmetry) and the third conformer with  $\tau = 180^\circ$  (C<sub>s</sub> symmetry) are less stable in energy by 0.43 and 0.92 kcal mol<sup>–1</sup>, respectively. The temperature of the measurements was 25 °C.

<sup>a)</sup> Three times the estimated standard errors.

<sup>b)</sup> Differences in the C–H bond lengths were assumed at the *ab initio* value.

<sup>c)</sup> Dependent parameter.

<sup>d)</sup> [ $r(\text{S–C(2)}) - r(\text{S–C(5)})$ ] and [ $r(\text{C(2)=C(3)}) - r(\text{C(4)=C(5)})$ ] were assumed at the *ab initio* value of 0.002 Å.

<sup>e)</sup> Assumed at the *ab initio* value.

Tanabe, M., Kuze, N., Takeuchi, H., Konaka, S.: J. Mol. Struct. **380** (1996) 205.

[II/25D \(3, 1972\)](#)