

667  
MW**C<sub>5</sub>H<sub>10</sub>S****Pentamethylene sulfide**  
Thiane  
Tetrahydro-2*H*-thiopyran**C<sub>s</sub> (chair)**

$r_s$	Å <sup>a)</sup>	$\theta_s$	deg <sup>a)</sup>
S–C( $\alpha$ )	1.8164(1)	C( $\alpha$ )–S–C( $\alpha'$ )	97.299(8)
C( $\alpha$ )–C( $\beta$ )	1.5156(1)	S–C( $\alpha$ )–C( $\beta$ )	112.733(9)
C( $\beta$ )–C( $\gamma$ )	1.5311(1)	C( $\alpha$ )–C( $\beta$ )–C( $\gamma$ )	112.407(9)
		C( $\beta$ )–C( $\gamma$ )–C( $\beta'$ )	112.956(9)
		$\phi^b$	130.64(2)
		$\phi^b$	127.19(2)

$r_0$	Å	$\theta_0$	deg
S–C( $\alpha$ )	1.812(6)	C( $\alpha$ )–S–C( $\alpha'$ )	97.8(4)
C( $\alpha$ )–C( $\beta$ )	1.533(8)	S–C( $\alpha$ )–C( $\beta$ )	112.5(5)
C( $\beta$ )–C( $\gamma$ )	1.534(6)	C( $\alpha$ )–C( $\beta$ )–C( $\gamma$ )	112.2(6)
C–H	1.095 <sup>c)</sup>	C( $\beta$ )–C( $\gamma$ )–C( $\beta'$ )	113(6)
		H–C–H	108.5 <sup>c)</sup>
		$\phi^b$	130.4(6)
		$\phi^b$	127(1)

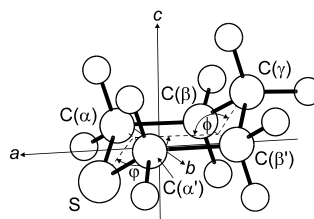
Atom	$a_s$ [Å]	$b_s$ [Å]	$c_s$ [Å]
S	1.42450	0.0	–0.17071
C( $\alpha'$ , $\alpha$ )	0.34338	±1.36349	0.35030
C( $\beta'$ , $\beta$ )	–1.04269	±1.27641	0.2564
C( $\gamma$ )	–1.78099	0.0	0.1560

Local C<sub>2v</sub> symmetry around the C atom was assumed.

<sup>a)</sup> Estimated standard errors.

<sup>b)</sup> See figure for the definition.

<sup>c)</sup> Assumed.



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Replaces [II/25D \(3, 2050\)](#), MW