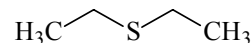


599
MW**C₄H₁₀S****Diethyl sulfide**
1,1'-Thiobisethane**C₂** (*gauche-gauche*)
C_{2v} (*anti-anti*)
C₁ (*anti-gauche*)

r_s	\AA^a		
	<i>anti-anti</i>	<i>anti-gauche</i>	<i>gauche-gauche</i>
C(1)–C(2)	1.529(5)	1.526(5)	1.519(7)
C(2)–S	1.805(2)	1.82(2)	1.809(6)
C(3)–S	1.805(2)	1.80(3)	1.809(6)
C(3)–C(4)	1.529(5)	1.519(6)	1.519(7)

θ_s	deg^a		
	<i>anti-anti</i>	<i>anti-gauche</i>	<i>gauche-gauche</i>
C(1)–C(2)–S	109.6(3)	110(1)	114.8(5)
C(2)–S–C(3)	99.3(1)	100(1)	101.6(3)
S–C(3)–C(4)	109.6(3)	115(1)	114.8(5)
C(1)–C(2)–S–C(3) ^b	0(3)	4(7)	65(1)
C(2)–S–C(3)–C(4) ^b	0(3)	71(3)	65(1)

<i>anti-anti</i>				<i>gauche-gauche</i>			
Atom	a_s [\AA]	b_s [\AA]	c_s [\AA]	a_s [\AA]	b_s [\AA]	c_s [\AA]	
C(1)	2.6995	−0.11	0.0	1.9242	−0.974	0.392	
C(2)	1.376	0.655	0.0	1.240	−0.11	−0.654	
S	0.0	−0.513	0.0	0.0	1.036	0.0	

<i>anti-gauche</i>			
Atom	a_s [\AA]	b_s [\AA]	c_s [\AA]
C(1)	2.5293	0.380	−0.08
C(2)	1.072	0.651	0.283
S	0.05	−0.784	−0.162
C(3)	−1.542	−0.256	0.480
C(4)	−2.2065	0.862	−0.304

Three conformers were detected.

^a) Uncertainties derived by error propagation from the standard errors.^b) Dihedral angle.Plusquellic, D.F., Suenram, R.D., Maté, B., Jensen, J.O., Samuels, A.C.: J. Chem. Phys. **115** (2001) 3057.