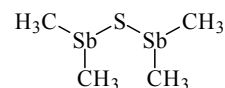


607  
ED, DFT  
calculations

$\text{C}_4\text{H}_{12}\text{SSb}_2$

**Thiobis[dimethylstibine]**  
Bis(dimethylstibino)sulfane

$\text{C}_2$  (near *syn-syn*)  
 $\text{C}_s$  (*syn-anti*)



$r_a$	$\text{\AA}^a$	$\theta_a$	$\text{deg}^a$
Sb–S	2.414(4)	S–Sb–C	92.6(6)
Sb–C	2.132(3)	C–Sb–C	95(3)
C–H(mean)	1.096(5)	Sb–C–H(mean)	110.0(6)
		near <i>syn-syn</i>	<i>syn-anti</i>
		Sb–S–Sb <sup>b)</sup>	98.7(5) 104.5(5)
		$\angle(\text{Sb–S–Sb–lp})$ <sup>c)</sup>	$\pm 33(4)$ 0 and 180 <sup>d)</sup>

Local  $\text{C}_{3v}$  symmetry was assumed for the  $\text{SbCH}_3$  groups, and one C–H bond of each methyl group was fixed to the *anti* position with respect to the S–Sb bond. The molecule was found to exist as a mixture of near *syn-syn* (52(4)%) and *syn-anti* (48(4)%) conformers. The energy difference between these conformers was estimated to be  $3.9 \text{ kJ mol}^{-1}$  by BPW91/LanL2DZ method.

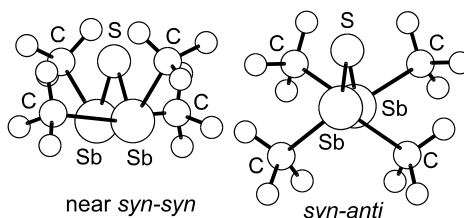
The nozzle temperature was 54(5) °C.

<sup>a)</sup> Twice the estimated standard errors including a systematic error.

<sup>b)</sup> Difference between the Sb–S–Sb angles of the two conformers was assumed at the DFT calculated value.

<sup>c)</sup> Zero degree for the *syn* position; lp is the lone pair on the Sb atom.

<sup>d)</sup> Assumed.



Haaland, A., Shorokhov, D.J., Volden, H.V., Breunig, H.J., Denker, M., Rösler, R.: Z. Naturforsch. **53b** (1998) 381.

See also: Haaland, A., Shorokhov, D.J., Sokolov, V.I., Volden, H.V., Breunig, H.J., Denker, M., Rösler, R.: Phosphorus Sulfur Silicon **136-138** (1998) 463.