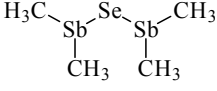


609 **C₄H₁₂Sb₂Se**
ED, DFT calculations

Bis(dimethylstibino)selane
Selenobis[dimethylstibine]
Bis(dimethylstibino) selenide

C₂ (near *syn-syn*)
C_s assumed (*syn-anti*)
(see also comment)

r_a	Å ^{a)}	θ_a	deg ^{a)}	
Sb–Se	2.551(5)	Se–Sb–C	95.0(7)	
Sb–C	2.152(7)	C–Sb–C	92(7)	
C–H (mean)	1.103(9)	Sb–C–H (mean)	109 ^{b)}	
<i>syn-syn</i>		<i>syn-syn</i>		
Sb...Sb ^{c)}	3.80(6)	Sb–Se–Sb	96.3(11)	
<i>syn-anti</i>		Sb–Se–Sb–lp ^{d)}	±26(3)	
Sb...Sb ^{c)}	3.96(6)	<i>syn-anti</i>		
		Sb–Se–Sb	101.9(11)	
		Sb–Se–Sb–lp ^{d)}	0, 180 ^{e)}	

The molecule exists as a near *syn-syn* conformer. The presence of the second conformer (*syn-anti*) was uncertain. The ED analysis yielded the mole fraction of the *syn-anti* conformer $x = 0.27(18)$. Local C_{3v} symmetry was assumed for the SbCH₃ groups. Methyl group orientations were assumed in such a way that one C–H bond is *anti* to the Sb–Se bond. BPW91/LanL2DZ+P calculations indicated the existence of *syn-anti* conformer 3.7 kJ mol^{–1} above the more stable near *syn-syn* conformer. The nozzle temperature was 70(5) °C.

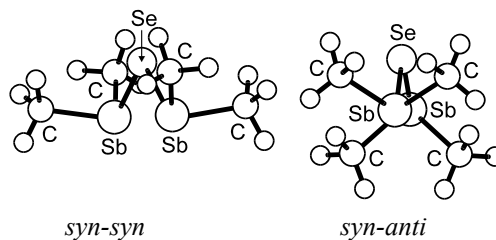
^{a)} Twice the estimated standard errors including a systematic error.

^{b)} Assumed at the value from BPW91/LanL2DZ+P calculations.

^{c)} Difference between Sb...Sb distances in the two conformers was assumed at the value from BPW91/LanL2DZ+P calculations.

^{d)} lp is the lone pair on the Sb atom.

^{e)} Assumed.



Haaland, A., Sokolov, V.I., Volden, H.V., Breunig, H.J., Denker, M., Rösler, R.: Z. Naturforsch. **52b** (1997) 296.

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.