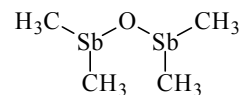


605 **C₄H₁₂OSb₂**
ED, DFT calculations

Bis(dimethylstibino) oxide
Oxybis[dimethylstibine]

C₂ (near *syn-syn*)
C_s assumed (*syn-anti*)

r_a	Å ^{a)}	θ_a	deg ^{a)}
Sb–O	1.976(14)	O–Sb–C	92.3(6)
Sb–C	2.144(9)	C–Sb–C	97.8(18)
C–H (mean)	1.108(7)	Sb–C–H (mean)	108.7(13)
<i>syn-syn</i>		<i>syn-syn</i>	
Sb...Sb ^{b)}	3.462(16)	Sb–O–Sb	122.3(16)
<i>syn-anti</i>		Sb–O–Sb–lp ^{c)}	±28(4)
Sb...Sb ^{b)}	3.597(16)	<i>syn-anti</i>	
		Sb–O–Sb	131.1(18)
		Sb–O–Sb–lp ^{c)}	0, 180 ^{d)}



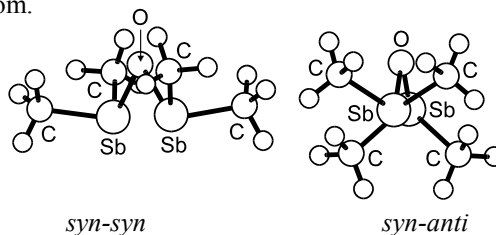
The molecule exists as a mixture of the near *syn-syn* (49(7)%) and *syn-anti* (51(7)%) conformers. Local C_{3v} symmetry was assumed for the SbCH₃ groups. Methyl group orientations were assumed in such a way that one C–H bond is *anti* to the Sb–O bond. BPW91/LanL2DZ+P calculations indicated the existence of *syn-anti* conformer 4.6 kJ mol^{–1} above the more stable near *syn-syn* conformer. The nozzle temperature was 22(2) °C.

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

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

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

^{d)} 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.