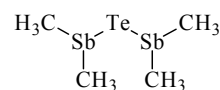


**610**      **C<sub>4</sub>H<sub>12</sub>Sb<sub>2</sub>Te**  
ED, DFT calculations

**Tellurobis[dimethylstibine]**  
Bis(dimethylstibino)tellurane

**C<sub>2</sub>** (near *syn-syn*)  
**C<sub>s</sub>** (*syn-anti*)



| $r_a$     | Å <sup>a)</sup> | $\theta_a$                           | deg <sup>a)</sup>                    |
|-----------|-----------------|--------------------------------------|--------------------------------------|
| Sb–Te     | 2.781(3)        | Te–Sb–C                              | 93.7(11)                             |
| Sb–C      | 2.172(5)        | C–Sb–C                               | 108(6)                               |
| C–H(mean) | 1.109(14)       | Sb–C–H(mean)                         | 112(2)                               |
|           |                 |                                      | near <i>syn-syn</i> <i>syn-anti</i>  |
|           |                 | Sb–Te–Sb <sup>b)</sup>               | 91(2)      96(2)                     |
|           |                 | $\angle$ (Sb–Te–Sb–lp) <sup>c)</sup> | $\pm 45(12)$ 0 and 180 <sup>d)</sup> |

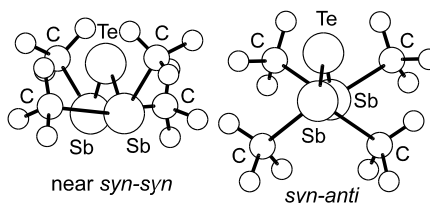
Local C<sub>3v</sub> symmetry was assumed for the SbCH<sub>3</sub> groups, one C–H bond of each methyl group was fixed to the *anti* position with respect to the S–Sb bond. The molecule was found to exist as a near *syn-syn* conformer (81(32)%), the presence of the *syn-anti* conformer was uncertain (19(32)%). The energy difference between near *syn-syn* and *syn-anti* conformers was estimated to be 0.9 kJ mol<sup>–1</sup> by BPW91/LanL2DZ method. The nozzle temperature was 96(2) °C.

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

<sup>b)</sup> Difference between the Sb–Te–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.