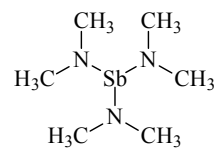
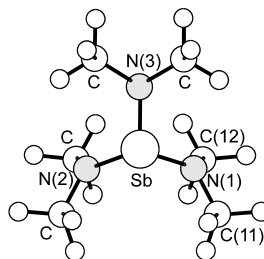


761 **C₆H₁₈N₃Sb**ED, *ab initio*
calculations**Tris(dimethylamino)sbaine****C_s**

r_a	Å ^{a)}	θ_a	deg ^{a)}
Sb–N(1,2)	2.022(12)	N(1)–Sb–N(2)	107.3(8)
Sb–N(3)	2.043(12) ^{b)}	N(1)–Sb–N(3)	94.7(8) ^{b)}
N(1,2)–C	1.450(7)	Sb–N(1)–C(11)	118.8(6)
N(3)–C	1.454(7) ^{b)}	Sb–N(1)–C(12)	123.2(6) ^{b)}
C–H (mean)	1.119(7) ^{c)}	Sb–N(3)–C	116.6(6) ^{b)}
		C–N(1,2)–C	116.7(6)
		C–N(3)–C	115.5(6) ^{b)}
		N–C–H (mean)	114.6(15) ^{c)}
		N(2)–Sb–N(1)–C(12)	54(3)
		lp–Sb–N(3)–lp ^{d)}	180 ^{e)}
		lp–Sb–N(1)–lp ^{d)}	78 ^{f)}
		lp–N(3)–Sb–N(1) ^{d)}	54 ^{f)}
		lp–N(1)–Sb–N(3) ^{d)}	54 ^{f)}
		lp–N(1)–Sb–N(2) ^{d)}	150 ^{f)}
		$\Sigma\alpha$ [N(1)] ^{g)}	359 ^{f)}
		$\Sigma\alpha$ [N(3)] ^{g)}	349 ^{f)}
		$\Sigma\alpha$ (Sb) ^{g)}	297 ^{f)}



According to *ab initio* calculations, the conformation with C₃ symmetry is significantly less stable than that with C_s symmetry ($\Delta E = 12.1 \text{ kJ mol}^{-1}$ (HF/6-31G*) and $\Delta E = 17.7 \text{ kJ mol}^{-1}$ (MP2/6-31G*)). The nozzle temperature was 20(3) °C.



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

^{b)} Dependent parameter. The differences [Sb–N(3)] – [Sb–N(1)], [N(3)–C] – [N(1)–C], [N(1)–Sb–N(3)] – [N(1)–Sb–N(2)], [Sb–N(1)–C(12)] – [Sb–N(1)–C(11)], [Sb–N(3)–C] – [Sb–N(1)–C(11)] and [C–N(3)–C] – [C–N(1)–C] were constrained to the values from HF/6-31G* calculations.

^{c)} Differences among the similar parameters were constrained to the values from HF/6-31G* calculations.

^{d)} lp denotes lone pair.

^{e)} Assumed according to the results of *ab initio* calculations.

^{f)} Dependent parameter.

^{g)} Sum of the valence angles at the N(1), N(3) and As atoms, respectively.

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See also: Belyakov, A.V., Baskakova, P.E., Haaland, A., Krannich, L.K., Swang, O.: Zh. Obshch. Khim. **67** (1997) 263; Russ. J. Gen. Chem. (Engl. Transl.) **67** (1997) 245.