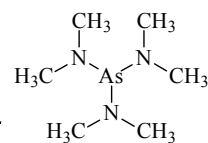


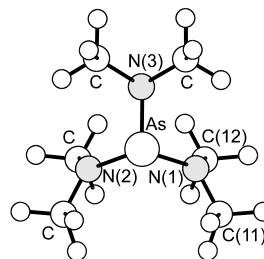
757 **C₆H₁₈AsN₃**ED, *ab initio*
calculations**Tris(dimethylamino)arsine**

Hexamethylarsenous triamide

C_s

r_a	Å ^{a)}	θ_a	deg ^{a)}
As–N(1,2)	1.849(5)	N(1)–As–N(2)	111.2(9)
As–N(3)	1.870(5) ^{b)}	N(1)–As–N(3)	100.3(9) ^{b)}
N(1,2)–C	1.455(4)	As–N(1)–C(11)	115.4(4)
N(3)–C	1.463(4) ^{b)}	As–N(1)–C(12)	122.8(4) ^{b)}
C–H (mean)	1.125(6) ^{c)}	As–N(3)–C	112.7(4) ^{b)}
		C–N(1,2)–C	115.4(4)
		C–N(3)–C	112.8(4) ^{b)}
		N–C–H (mean)	113.6(11) ^{c)}
		N(2)–As–N(1)–C(12)	46(3)
		lp–As–N(3)–lp ^{d)}	180 ^{e)}
		lp–As–N(1)–lp ^{d)}	82 ^{f)}
		lp–N(3)–As–N(1) ^{d)}	57 ^{f)}
		lp–N(1)–As–N(3) ^{d)}	45 ^{f)}
		lp–N(1)–As–N(2) ^{d)}	150 ^{f)}
		$\Sigma\alpha$ [N(1)] ^{g)}	353 ^{f)}
		$\Sigma\alpha$ [N(3)] ^{g)}	338 ^{f)}
		$\Sigma\alpha$ (As) ^{g)}	312 ^{f)}

According to *ab initio* calculations, the conformation with C₃ symmetry is significantly less stable than that with C_s symmetry ($\Delta E = 23.2 \text{ kJ mol}^{-1}$ (HF/6-31G*) and $\Delta E = 30.4 \text{ kJ mol}^{-1}$ (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 [As–N(3)] – [As–N(1)], [N(3)–C] – [N(1)–C], [N(1)–As–N(3)] – [N(1)–As–N(2)], [As–N(1)–C(12)] – [As–N(1)–C(11)], [As–N(3)–C] – [As–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.

Baskakova, P.E., Belyakov, A.V., Colacot, T., Krannich, L.K., Haaland, A., Volden, H.V., Swang, O.: J. Mol. Struct. **445** (1998) 311.

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.