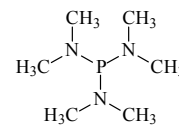
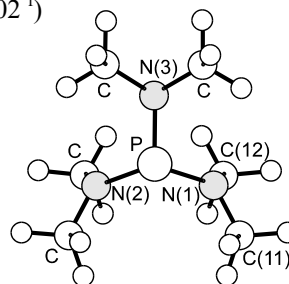


**760**      **C<sub>6</sub>H<sub>18</sub>N<sub>3</sub>P**ED, *ab initio*  
calculations**Tris(dimethylamino)phosphine**Hexamethylphosphorous triamide  
Tris(dimethylamino)phosphane**C<sub>s</sub>**

$r_a$	$\text{\AA}^a$	$\theta_a$	deg <sup>a)</sup>
P–N(1,2)	1.703(6)	N(1)–P–N(2)	108.3(6)
P–N(3)	1.738(6) <sup>b)</sup>	N(1)–P–N(3)	96.8(6) <sup>b)</sup>
N(1,2)–C	1.466(6)	P–N(1)–C(11)	116.5(5)
N(3)–C	1.473(6) <sup>b)</sup>	P–N(1)–C(12)	124.1(5) <sup>b)</sup>
C–H (mean)	1.126(6) <sup>c)</sup>	P–N(3)–C	113.6(5) <sup>b)</sup>
		C–N(1,2)–C	112.5(5)
		C–N(3)–C	109.4(5) <sup>b)</sup>
		N–C–H (mean)	110.6(8) <sup>c)</sup>
		N(2)–P–N(1)–C(12)	65(6)
		lp–P–N(3)–lp <sup>d)</sup>	180 <sup>e)</sup>
		lp–P–N(1)–lp <sup>d)</sup>	59 <sup>f)</sup>
		lp–N(3)–P–N(1) <sup>d)</sup>	55 <sup>f)</sup>
		lp–N(1)–P–N(3) <sup>d)</sup>	71 <sup>f)</sup>
		lp–N(1)–P–N(2) <sup>d)</sup>	171 <sup>f)</sup>
		$\Sigma\alpha[\text{N}(1)]$ <sup>g)</sup>	353 <sup>f)</sup>
		$\Sigma\alpha[\text{N}(3)]$ <sup>g)</sup>	337 <sup>f)</sup>
		$\Sigma\alpha(\text{P})$ <sup>g)</sup>	302 <sup>f)</sup>

According to *ab initio* calculations, the conformation with C<sub>3</sub> symmetry is significantly less stable than that with C<sub>s</sub> symmetry ( $\Delta E = 21.9 \text{ kJ mol}^{-1}$  (HF/6-31G\*) and  $\Delta E = 27.6 \text{ kJ mol}^{-1}$  (MP2/6-31G\*). Conclusion about C<sub>s</sub> symmetry of the molecule does not agree with the results of [1] (C<sub>3</sub> symmetry). The nozzle temperature was 20(3) °C.



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

<sup>b)</sup> Dependent parameter. The differences [P–N(3)] – [P–N(1)], [N(3)–C] – [N(1)–C], [N(1)–P–N(3)] – [N(1)–P–N(2)], [P–N(1)–C(12)] – [P–N(1)–C(11)], [P–N(3)–C] – [P–N(1)–C(11)] and [C–N(3)–C] – [C–N(1)–C] were constrained to the values from HF/6-31G\* calculations.

<sup>c)</sup> Differences among the similar parameters were constrained to the values from HF/6-31G\* calculations.

<sup>d)</sup> lp denotes lone pair.

<sup>e)</sup> Assumed according to the results of *ab initio* calculations.

<sup>f)</sup> Dependent parameter.

<sup>g)</sup> Sum of the valence angles at the N(1), N(3) and P atoms, respectively.

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See also: Belyakov, A.V., Baskakova, P.E., Haaland, A., Swang, O., Vilkov, L.V., Golubinskii, A.V., Bogoradovskii, E.T.: Zh. Obshch. Khim. **68** (1998) 269; Russ. J. Gen. Chem. (Engl. Transl.) **68** (1998) 244.

[1] Vilkov, L.V., Khaikin, L.S., Evdokimov, V.V.: Zh. Strukt. Khim. **13** No.1 (1972) 7; J. Struct. Chem. (Engl. Transl.) **13** (1972) 4.

Replaces [II/25D \(3, 2390\)](#)