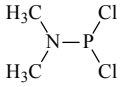
295 **$C_2H_6Cl_2NP$** **Dimethylphosphoramidous dichloride** **C_1** assumed (*gauche*)

ED, *ab initio* calculations

Dichloro(dimethylamino)phosphine



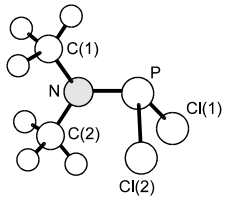
r_{h1} [a])	Å [b])	θ_{h1} [a])	deg [b])
P–N	1.668(4)	Cl–P–Cl	97.2(1)
N–C(1) [c])	1.454(3)	N–P–Cl(1)	100.9(3)
N–C(2) [c])	1.449(3)	N–P–Cl(2)	103.3(3)
P–Cl(1)	2.074(5)	C–N–C	112.6(6)
P–Cl(2)	2.111(5)	P–N–C(1)	115.0(4)
C–H [d])	1.093(3)	P–N–C(2)	125.9(4)
		C(1)–N–P–Cl(1)	–152.8(15)
		C(1)–N–P–Cl(2)	107.0(14)
		C(2)–N–P–Cl(1)	57.6(24)
		C(2)–N–P–Cl(2)	–42.6(24)

The amino group was found to be nonplanar.

The temperature of the measurements was *ca*. 325 K.

In an earlier ED study [1] (at the nozzle temperature of 22(3) °C), the bond configuration at the N atom was found to be nearly planar. According to the results of B3PW91/6-311+G* calculations [1], the conformer of C_1 symmetry is the most stable conformation but the transition state of the molecule of C_s symmetry with orthogonal lone pairs (τ(lp–N–P–lp) = 90°) and a strictly planar bond configuration at the N atom lies only 0.25 kcal mol^{-1} above the equilibrium structure.

[a]) Nonlinear kinematic effect was taken into account.
[b]) Estimated standard errors including a systematic error.
[c]) Difference between the N–C bond lengths was assumed at the value from MP2/6-31G** calculations.
[d]) Average value.



Khaikin, L.S., Grikina, O.E., Kramarenko, S.S., Zhilinskaya, E.A., Zhilinskii, B.I.: Izv. Akad. Nauk, Ser. Khim. **9** (2001) 1475; Russ. Chem. Bull. (Engl. Transl.) **50** (2001) 1550.

[1] Baskakova, P.E., Belyakov, A.V., Haaland, A., Volden, H.V.: J. Mol. Struct. **567-568** (2001) 197.

Replaces II/25B(**3**, 862)