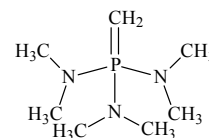


817 **C₇H₂₀N₃P**ED, *ab initio*
calculations***N,N,N',N'',N''',N'''*-Hexamethyl-
1-methylenephosphoranetriamine**

Tris(dimethylamino)methylenephosphorane

Tris(dimethylamino)methylene- λ^5 -phosphane**C_s** assumed

r_a	Å ^{a)}	θ_a	deg ^{a)}
P=C	1.620(5)	N(1,2)–P–N(3)	97.0(5)
P–N(1,2)	1.684(3)	N(1)–P–N(2)	115.2(13)
P–N(3)	1.718(6)	C=P–N(1,2)	110.0(5)
N(1,2)–C	1.457(3)	C=P–N(3)	127.1(8)
N(3)–C	1.461(6)	P–N–C(11,21)	121.9(7)
C–H ^{b)}	1.115(1)	P–N–C(12,22)	122.6(7)
		P–N(3)–C	111.4(5)
		C–N(1,2)–C	115.0(5)
		C–N(3)–C	110.1(10)
		N–C–H ^{b)}	111.1(3)
		P=C–H	118.1 ^{c)}
		H–C–H	117.6 ^{c)}
		$\Sigma\alpha(N(1),N(2))$ ^{d)}	359.5(11)
		$\Sigma\alpha(N(3))$ ^{d)}	332.9(13)
		τ_1 ^{e)}	$\pm 1.5(18)$
		τ_2 ^{f)}	$\pm 178.4(21)$



Local C₂ symmetry of the N(CH₃)₂ groups and local C_{3v} symmetry of the NCH₃ groups were assumed. The ED analysis was carried out by applying flexible restraints based on the results of MP2/6-31G* calculations. The following results were obtained for the methyl conformation: in the position that NMe₂ has C_{2v} symmetry, one C–H bond is staggered with respect to the further N–C bond of the NMe₂ group. The two CH₃ groups are twisted about their respective N–C bonds by 20.3(24)°.

The nozzle was at 140 °C.

^{a)} Estimated standard errors.

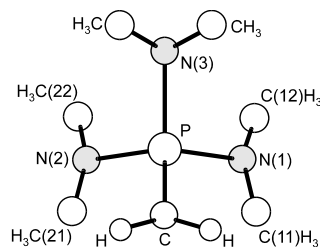
^{b)} Mean value.

^{c)} Assumed at the value from MP2/6-31G* calculations.

^{d)} Sum of the angles at the N atoms.

^{e)} C=P–N–C(11,21) torsional angles from the *syn* position.

^{f)} C=P–N–C(12,22) torsional angles from the *syn* position.



Mitzel, N.W., Smart, B.A., Dreihäupl, K.-H., Rankin, D.W.H., Schmidbaur, H.: J. Am. Chem. Soc. **118** (1996) 12673.