

1413
MW

C₃H₉P

Trimethylphosphine

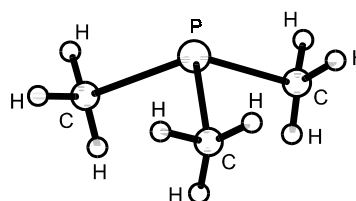
C_{3v}
P(CH₃)₃

r_0	Å	θ_0	deg
C–H(s), C–H(a)	1.096(1)	P–C–H(s)	111.6(3)
P–C	1.845(1)	P–C–H(a)	109.1(2)
		H(s)–C–H(a), H(a)–C–H(a)	109.0(2)
		C–P–C	98.9(2)

Chatterjee, K.K., Durig, J.R., Bell, S.: J. Mol. Struct. **265** (1992) 25.

r_s	Å	θ_s	deg
C–H(s)	1.112(5)	P–C–H(s)	111.4(3)
C–H(a)	1.090(10)	P–C–H(a)	109.8(4)
P–C	1.843(5)	H(s)–C–H(a)	108.2(8)
H(a)...H(a)	1.763(15)	H(a)–C–H(a)	109.4(4)
		C–P–C	98.9(2)

Atom	a_s [Å]	b_s [Å]	c_s [Å]
P	0.0	0.0	0.5514
C	1.6174	0.0	–0.3378
H(s)	1.4771	0.0	–1.4307
H(a)	2.1809	±0.8816	–0.0979



The methyl groups are staggered with respect to the opposite P–C bonds.

Bryan, P.S., Kuczkowski, R.L.: J. Chem. Phys. **55** (1971) 3049.

See also: Lide, D.R., Mann, D.E.: J. Chem. Phys. **29** (1958) 914.

ED

[1]			
r_g	Å ^{b)}	$\theta^a)$	deg ^{b)}
C–H	1.091(6)	P–C–H	110.7(5)
P–C	1.8465(30)	C–P–C	98.6(3)
C...C	2.800(5)		

The methyl groups are staggered with respect to the opposite P–C bonds. The barrier to rotation of the methyl groups ≥ 1 kcal/mol.

The nozzle temperature was not given, probably room temperature.

^{a)} Unidentified, possibly θ_a .

^{b)} Estimated standard errors.

[2]			
r_α^0	Å ^{a)}	θ_α^0	deg ^{a)}
C–H	1.070(6)	P–C–H	111.4(5)
P–C	1.844(3)	C–P–C	98.8(3)

Vibrational corrections are applied to the experimental data published in [1].

^{a)} Estimated standard errors.

[1] Bartell, L.S., Brockway, L.O.: J. Chem. Phys. **32** (1960) 512.

[2] Beagley, B., Medwid, A.R.: J. Mol. Struct. **38** (1977) 229.