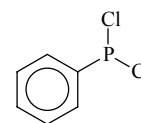
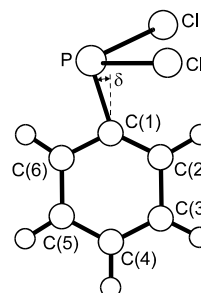


709 **C₆H₅Cl₂P**ED, *ab initio*
calculations**Phenylphosphonous dichloride**

Dichlorophenylphosphine

C_s

r_a	\AA^a	θ_a	deg^a
P–Cl	2.060(3)	C–P–Cl	100.5(5)
P–C	1.823(5)	Cl–P–Cl	100.2(5)
C–C ^{b)}	1.396(2)	C–C(1)–C	121.2(9)
C–H	1.098(9)	C–C(2)–C	119.5(8)
		C–C(6)–C	119.8(8)
		C–C(3)–C	118.2 ^{c)}
		C–C(4)–C	123.3 ^{c)}
		C–C(5)–C	117.8 ^{c)}
		δ^d	5.0(5)



The structural parameters and parameters of the potential function were refined by taking into account the relaxation of the molecular geometry estimated by the HF/6-31G** method. The internal rotation potential was found to have a minimum at $\tau = 0^\circ$ (τ is the angle between the bisector of the Cl–P–Cl angle and the plane of the benzene ring) and a two-fold barrier height (V_2) of 1.24(54) kcal mol^{–1}. The nozzle temperature was 25 °C.

^{a)} Three times the estimated standard errors including a systematic error.

^{b)} Average value.

^{c)} Dependent parameter.

^{d)} Angle between the P–C bond and the bisector of the C–C(1)–C angle.

Novikov, V.P., Samdal, S., Vilkov, L.V.: J. Mol. Struct. **413-414** (1997) 279.

Replaces [II/25D \(3, 2196\)](#)