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(2-Chlorophenyl)diphenylphosphine

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Key indicators

Single-crystal X-ray study

T = 295 K

Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$

R factor = 0.039

wR factor = 0.115

Data-to-parameter ratio = 19.2

For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

The crystal structure of (2-chlorophenyl)diphenylphosphine, $\text{C}_{18}\text{H}_{14}\text{ClP}$, has been determined at 295 (1) K. The conformation of the molecule is similar to that of the analogous 2-bromo and 2-methyl compounds.

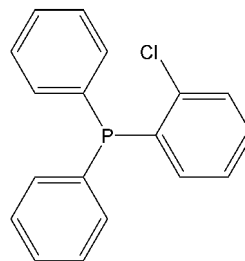
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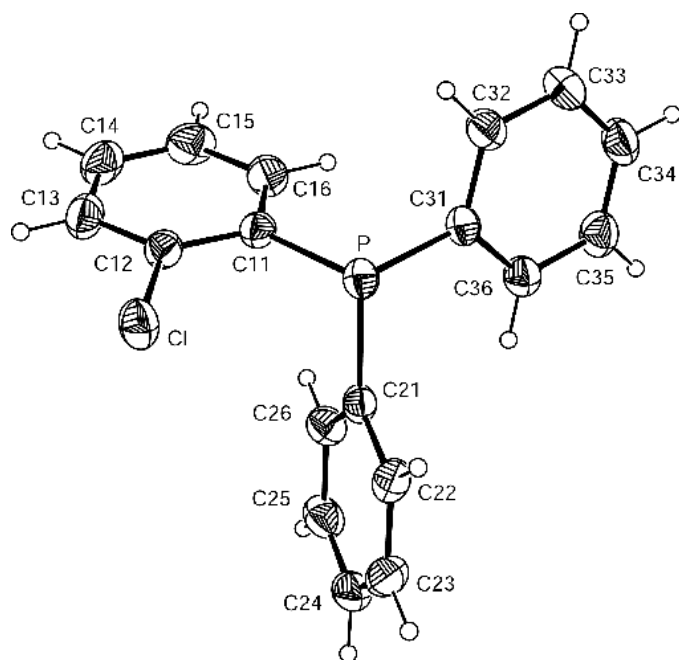
Comment

(2-Chlorophenyl)diphenylphosphine, (I), has been shown to coordinate to a range of metal centres either as a monodentate ligand through the P-donor atom or as a chelating ligand through both the phosphorus and the aryl chloride donor atoms (Burk *et al.*, 1988; Lahuerta *et al.*, 1988, Coalter *et al.*, 2000). The solid-state structure of (I) (Fig. 1 and Table 1) is similar to that found for (2-bromophenyl)diphenylphosphine, (II) (Williams *et al.*, 2002), and (2-methylphenyl)diphenylphosphine, (III) (Bowmaker *et al.*, 1987), consisting of discrete molecular species linked in the crystal lattice through edge-to-face $\text{C}-\text{H}\cdots\pi$ interactions between the phenyl groups (Scudder & Dance, 1998). In accord with previous studies which demonstrate the poor hydrogen-bond acceptor properties of $\text{C}-\text{Cl}$ bonds (Aullón *et al.*, 1998), there is no evidence of significant $\text{C}-\text{H}\cdots\text{Cl}$ intermolecular interactions, with the shortest $\text{H}\cdots\text{Cl}$ distances $> 3.0 \text{ \AA}$.



(I)

Within each molecule, the chlorine is located *cis* to the phosphorus lone pair. The molecule adopts a propeller-shaped conformation with the phenyl rings twisted away from the pseudo-threefold axis through the P atom by 48, 22 and 49° [*cf.* 36, 27 and 53° in (II); 36, 27 and 53° in (III)]. The P–C bond lengths [mean value 1.835 (5) Å] and C–P–C bond angles [mean value 102.0 (2)°] are similar to those recorded for the ‘parent’ triphenylphosphine ligand [1.831 (2) Å and 101.9 (8)°; Dunne & Orpen, 1991]. Introduction of the chloro substituent results in a small increase in the P–C11–C12 angle to 118.7 (2)°, compared to 118.0 (2) and 117.1 (2)° for P–C21–C22 and P–C31–P32, respectively.

**Figure 1**

Plot of the title compound, showing the atom-numbering scheme (Farrugia, 1997). Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

Experimental

The title compound was prepared as a white powder by the reaction of chlorodiphenylphosphine with the Grignard reagent formed from *o*-bromochlorobenzene (Hart, 1960); m.p. 377–380 K. Crystals suitable for X-ray diffraction studies were obtained by recrystallization from benzene.

Crystal data

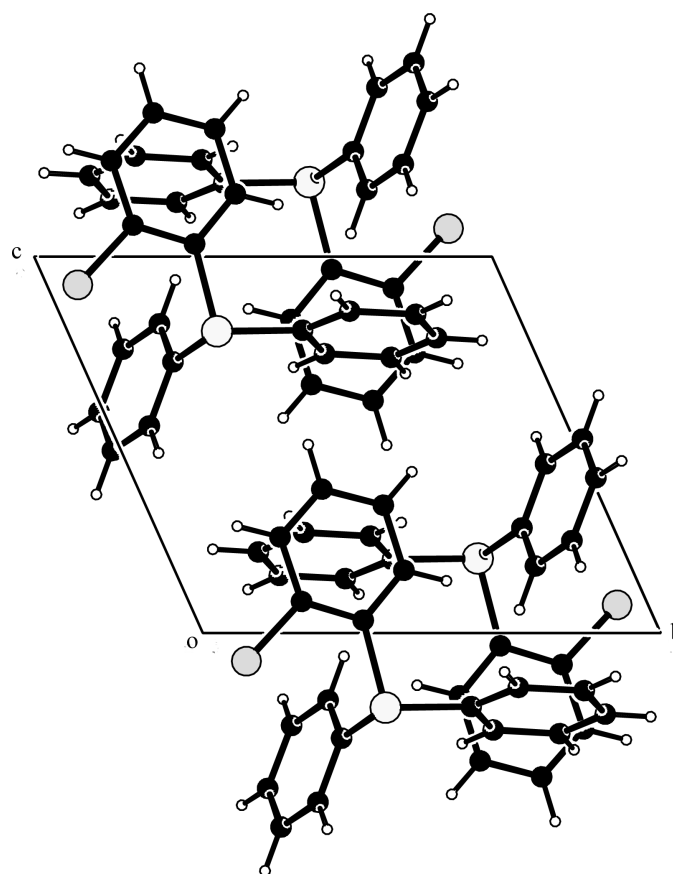
$C_{18}H_{14}ClP$	$Z = 2$
$M_r = 296.71$	$D_x = 1.293 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 10.646 (8) \text{ \AA}$	Cell parameters from 25 reflections
$b = 10.702 (6) \text{ \AA}$	$\theta = 12.6\text{--}16.6^\circ$
$c = 8.530 (6) \text{ \AA}$	$\mu = 0.34 \text{ mm}^{-1}$
$\alpha = 105.53 (6)^\circ$	$T = 295 \text{ K}$
$\beta = 99.88 (6)^\circ$	Prismatic, colorless
$\gamma = 119.27 (4)^\circ$	$0.30 \times 0.30 \times 0.30 \text{ mm}$
$V = 762.1 (11) \text{ \AA}^3$	

Data collection

Rigaku AFC-7R diffractometer	$\theta_{\text{max}} = 27.5^\circ$
ω - 2θ scans	$h = -13 \rightarrow 13$
Absorption correction: none	$k = -13 \rightarrow 13$
4248 measured reflections	$l = -6 \rightarrow 11$
3483 independent reflections	3 standard reflections
2452 reflections with $I > 2\sigma(I)$	every 150 reflections
$R_{\text{int}} = 0.021$	intensity decay: 1.8%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0519P)^2 + 0.1312P]$
$R[F^2 > 2\sigma(F^2)] = 0.039$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.115$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.04$	$\Delta\rho_{\text{max}} = 0.36 \text{ e \AA}^{-3}$
3483 reflections	$\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$
181 parameters	
H-atom parameters constrained	

**Figure 2**

The molecular packing in the crystal structure of (I). (Spek, 2001)

Table 1

Selected geometric parameters (\AA , $^\circ$).

Cl—C12	1.760 (3)	P—C21	1.834 (3)
P—C11	1.840 (2)	P—C31	1.830 (3)
C11—P—C21	100.23 (11)	Cl—C12—C13	117.0 (2)
C11—P—C31	102.47 (10)	P—C21—C22	118.0 (2)
C21—P—C31	103.26 (12)	P—C21—C26	123.65 (15)
P—C11—C12	118.67 (16)	P—C31—C32	117.1 (2)
P—C11—C16	124.73 (18)	P—C31—C36	124.68 (17)
Cl—C12—C11	119.92 (17)		

H atoms were located at calculated positions with C—H set to 0.95 \AA and constrained in the refinement.

Data collection: *MSC/AFC-7 Diffractometer Control Software* for Windows (Molecular Structure Corporation, 1999); cell refinement: *MSC/AFC-7 Diffractometer Control Software* for Windows; data reduction: *TEXSAN* (Molecular Structure Corporation, 2001); program(s) used to solve structure: *TEXSAN*; program(s) used to refine structure: *TEXSAN* and *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *PLATON* (Spek, 2001); software used to prepare material for publication: *TEXSAN* and *PLATON*.

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