

Michael L. Williams,
Cassandra L. Noack, Rodney J.
Saverin and Peter C. Healy*School of Science, Griffith University, Nathan,
Brisbane 4111, Australia

Correspondence e-mail: p.healy@sct.gu.edu.au

Key indicators

Single-crystal X-ray study

T = 295 K

Mean $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$

R factor = 0.043

wR factor = 0.150

Data-to-parameter ratio = 19.5

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

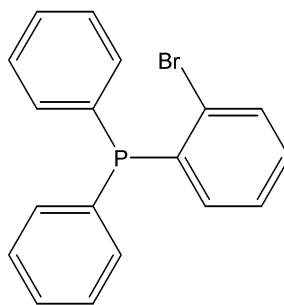
(2-Bromophenyl)diphenylphosphine

The crystal structure of (2-bromophenyl)diphenylphosphine, $\text{C}_{18}\text{H}_{14}\text{BrP}$, (I), has been determined at 295 (1) K. The structure of (I) is isomorphous with the analogous methyl compound (2-methylphenyl)diphenylphosphine.

Received 6 February 2002
Accepted 12 February 2002
Online 22 February 2002

Comment

(2-Bromophenyl)diphenylphosphine, (I), has been shown to coordinate to metal centres as both a monodentate ligand through the P-donor atom, and as a chelating hemilabile ligand through both the phosphine and the aryl bromide donor groups (Burk *et al.*, 1988). The solid-state structure of (I) is isomorphous with the structure reported for (2-methylphenyl)diphenylphosphine, (II) (Bowmaker *et al.*, 1987).



(I)

The structure consists of discrete molecular species which adopt a propeller-shaped conformation with the phenyl rings twisted away from the normal to the base of the PC_3 pyramid by 36, 27 and 53° [*cf.* (II): 36, 26 and 47°]. The bromide is located *cis* to the phosphorus lone pair. The P–C bond lengths [mean value 1.836 (6) Å] are similar to those recorded for triphenylphosphine [mean value 1.831 (2) Å; Dunne & Orpen, 1991], while the mean value of the C–P–C bond angles, 101.9 (8)°, is marginally smaller than the value of 102.8 (5)° observed for triphenylphosphine. Introduction of the bromo substituent on ring 1 in (I) results in a small increase in the P–C11–C12 angle to 119.8 (3)° compared to 117.1 (3) and 116.4 (3)° for P–C21–C22 and P–C31–C32. The corresponding angles in triphenylphosphine are 116.6 (1), 116.8 (1) and 117.5 (1)°. The molecules are linked in the crystal lattice through edge-to-face C–H... π interactions between the phenyl groups (Scudder & Dance, 1998). In accord with previous studies demonstrating the poor hydrogen-bond acceptor properties of C–X bonds (Aullón *et al.*, 1998), there is no evidence of significant C–H...Br intermolecular interactions in (I), with the shortest H...Br distances being greater than 3.1 Å.

Experimental

The title compound was obtained as a white crystalline powder from the $\text{PdCl}_2(\text{CH}_3\text{CN})_4$ -catalysed reaction between *ortho*-bromiodobenzene and diphenyl(trimethylsilyl)phosphine (Tunney *et al.*, 1987); m.p. 386–388 K. Crystals of the compound suitable for X-ray diffraction studies were obtained during an attempt to recrystallize the 1:2 copper(I) bromide complex by diffusion of ether into a solution of the complex in dichloromethane.

Crystal data

$\text{C}_{18}\text{H}_{14}\text{BrP}$	$D_x = 1.472 \text{ Mg m}^{-3}$
$M_r = 341.16$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 25 reflections
$a = 10.371 (5) \text{ \AA}$	$\theta = 13.2\text{--}16.0^\circ$
$b = 8.9735 (19) \text{ \AA}$	$\mu = 2.76 \text{ mm}^{-1}$
$c = 16.556 (6) \text{ \AA}$	$T = 295 (1) \text{ K}$
$\beta = 92.33 (4)^\circ$	Plate, colourless
$V = 1539.5 (10) \text{ \AA}^3$	$0.40 \times 0.30 \times 0.20 \text{ mm}$
$Z = 4$	

Data collection

Rigaku AFC-7R diffractometer	$R_{\text{int}} = 0.033$
ω - 2θ scans	$\theta_{\text{max}} = 27.5^\circ$
Absorption correction: ψ scan (North <i>et al.</i> , 1968)	$h = -13 \rightarrow 13$
$T_{\text{min}} = 0.383$, $T_{\text{max}} = 0.576$	$k = -11 \rightarrow 0$
4223 measured reflections	$l = -12 \rightarrow 21$
3540 independent reflections	3 standard reflections every 150 reflections
1823 reflections with $I > 2\sigma(I)$	intensity decay: 0.8%

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 1.0428P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.150$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.79 \text{ e \AA}^{-3}$
3540 reflections	$\Delta\rho_{\text{min}} = -0.70 \text{ e \AA}^{-3}$
182 parameters	Extinction correction: <i>SHELXL97</i>
H-atom parameters constrained	Extinction coefficient: 0.0033 (9)

Table 1

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

Br—C12	1.905 (5)	P—C21	1.833 (4)
P—C11	1.844 (4)	P—C31	1.832 (4)
C11—P—C21	101.51 (18)	Br—C12—C13	117.7 (3)
C11—P—C31	101.32 (18)	P—C21—C22	117.2 (3)
C21—P—C31	102.83 (16)	P—C21—C26	124.7 (3)
P—C11—C12	119.8 (3)	P—C31—C32	116.4 (3)
P—C11—C16	123.1 (3)	P—C31—C36	125.1 (3)
Br—C12—C11	120.8 (3)		

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

Data collection: *MSC/AFC-7 Diffractometer Control Software* (Molecular Structure Corporation, 1999); cell refinement: *MSC/AFC-7 Diffractometer Control Software*; data reduction:

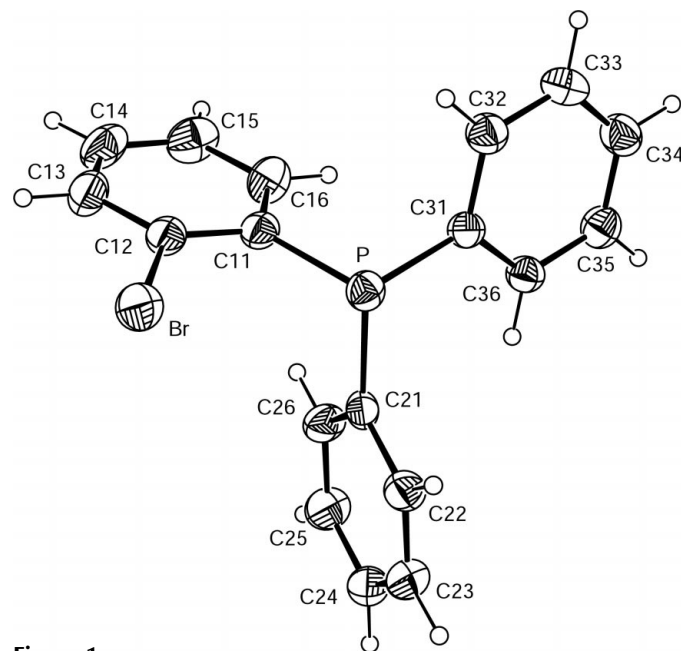


Figure 1

ORTEP-3 (Farrugia, 1997) plot of the title compound, showing the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

TEXSAN for Windows (Molecular Structure Corporation, 2001); program(s) used to solve structure: *TEXSAN* for Windows; program(s) used to refine structure: *TEXSAN* for Windows and *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *TEXSAN* and *PLATON* (Spek, 2001).

References

- Aullón, G., Bellamy, D., Brammer, L., Bruton, E. A. & Orpen, A. G. (1998). *Chem. Commun.* pp. 653–654.
- Bowmaker, G. A., Engelhardt, L. M., Healy, P. C., Kildea, J. D., Papsergio, R. I. & White, A. H. (1987). *Inorg. Chem.* **26**, 3533–3538.
- Burk, M. J., Crabtree, R. H. & Holt, E. M. (1988). *J. Organomet. Chem.* **341**, 495–509.
- Dunne, B. J. & Orpen, A. G. (1991). *Acta Cryst.* **C47**, 345–347.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Molecular Structure Corporation (1999). *MSC/AFC-7 Diffractometer Control Software* for Windows. Version 1.02. MSC, 9009 New Trails Drive, The Woodlands, TX 77381, USA.
- Molecular Structure Corporation (2001). *TEXSAN* for Windows. Version 1.06. MSC, 9009 New Trails Drive, The Woodlands, TX 77381, USA.
- North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.
- Scudder, M. & Dance, I. (1998). *J. Chem. Soc. Dalton Trans.* pp. 3155–3165.
- Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
- Spek, A. L. (2001). *PLATON* for Windows. Version 121201. University of Utrecht, The Netherlands.
- Tunney, S. E. & Stille, J. K. (1987). *J. Org. Chem.* **52**, 748–753.