C4—O1—C2	91.2 (1)	C4—C3—C24	115.3 (2)
O1—C2—C5	112.0 (2)	O19—C3—C2	114.3 (2)
O1—C2—C3	89.7 (1)	C4—C3—C2	84.1 (2)
C5—C2—C3	117.6 (2)	C24—C3—C2	114.7 (2)
O19—C3—C4	117.2 (2)	O1—C4—C3	91.2 (1)
O19—C3—C24	109.5 (2)		

For both compounds, data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1992); cell refinement: *CAD-4 EXPRESS*; data reduction: own programs; program(s) used to solve structures: *SHELXS*86 (Sheldrick, 1990*a*); program(s) used to refine structures: *SHELXL*93 (Sheldrick, 1993); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990*b*); software used to prepare material for publication: *SHELXL*93.

Lists of structure factors, least-squares-planes data, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: JZ1113). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Bach, T. (1995*a*). *Liebigs Ann. Chem.* pp. 855–866, and references therein.
Bach, T. (1995*b*). *Liebigs Ann. Chem.* pp. 1045–1053.
Bach, T., Jödicke, K., Kather, K. & Hecht, J. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 2271–2273.
Enraf–Nonius (1992). *CAD-4 EXPRESS.* Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Freilich, S. C. & Peters, K. S. (1981). *J. Am. Chem. Soc.* **103**, 6255–6257.
George, C. & Gilardi, R. (1986). *Acta Cryst.* C**42**, 1161–1164.
Holan, G., Kowala, C. & Wunderlich, J. A. (1973). *J. Chem. Soc. Chem. Commun.* p. 34.
Hospital, M., Leroy, F., Bats, J. P. & Moulines, J. (1978). *Cryst. Struct. Commun.* **7**, 309–311.
Khan, N., Morris, T. H., Smith, E. H. & Walsh, R. (1991). *J. Chem. Soc. Perkin Trans.* 1, pp. 865–870.
Luger, P. & Buschmann, J. (1984). *J. Am. Chem. Soc.* **106**, 7118–7121.
Mastryukov, V. S., Dorofeeva, O. V., Vilkov, L. V. & Hargittai, I. (1976). *J. Mol. Struct.* **34**, 99–112.
Morris, T. H., Smith, E. H. & Walsh, R. (1987). *J. Chem. Soc. Chem. Commun.* pp. 964–965.
Seitz, T., Muth, A., Huttner, G., Klein, T., Walter, O., Fritz, M. & Zsolnai, L. (1994). *J. Organomet. Chem.* **469**, 155–162.
Sheldrick, G. M. (1990*a*). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1990*b*). *SHELXTL-Plus. An Integrated System for Solving, Refining and Displaying Crystal Structures from Diffraction Data.* University of Göttingen, Germany.
Sheldrick, G. M. (1993). *SHELXL*93. *Program for the Refinement of Crystal Structures.* University of Göttingen, Germany.
Sutton, L. E. (1965). *Tables of Interatomic Distances and Configuration of Molecules and Ions,* pp. 1956–1959, Supplement. London: The Chemical Society.

(Pentafluorophenyl)diphenylphosphine

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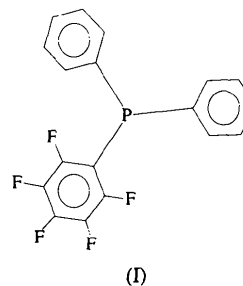
Abstract

In solid $C_{18}H_{10}F_5P$ the average P—C distance and C—P—C angle are 1.838 (2) Å and 102.9 (1)°, respectively. Intermolecular C—H···F hydrogen bonds and short F···F contacts are observed.

Comment

The title compound [(I), Fig. 1] has the expected geometry: the three P—C bonds are folded back from the lone-pair site, giving a slightly distorted tetrahedral geometry and C—P—C angles less than 109.5°.

(I)

The mean P—C bond length [1.838 (2) Å] is comparable with values of 1.828 (3) and 1.831 (2) Å for PPh_3 (Dunne & Orpen, 1991; Daly, 1964) and with the mean value of 1.828 Å for 2239 metal complexes containing PPh_3 (Orpen *et al.*, 1989). P—C12 is short [1.827 (2) Å] compared with P—C6 [1.846 (2) Å] and P—C18 [1.840 (2) Å]. A similar trend was observed in $[(\eta^6\text{-}C_6H_6)Cr(C_6F_5PPh_2)]_2Rh(CO)Cl$ (Faggiani, Hao, Lock, Sayer & McGlinchey, 1983). The average C—C distances are 1.375 (4) Å for the pentafluorophenyl ring and 1.382 (4) and 1.383 (4) Å for the two phenyl rings (C7–C12 and C13–C18).

The molecules are packed so that the lone pair of each P atom points along the shortest axis (*b* axis), a feature also observed in (2-methoxyphenyl)diphenylphosphine

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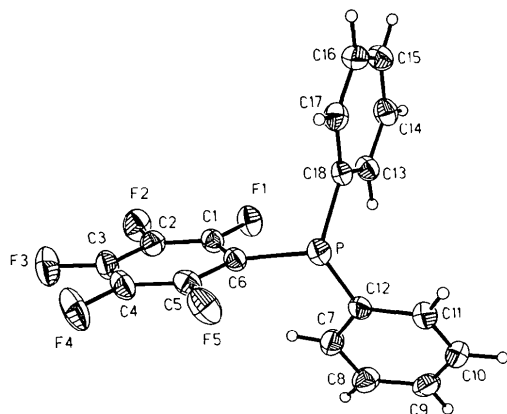
Fig. 1. 30% Thermal ellipsoid plot of the molecule with the numbering scheme.

(Shawkataly, Sivakumar & Fun, 1996). Four C—H···F hydrogen bonds are present: C7···F4^i 3.298 (3) Å, C7—H7···F4^i 123 (2)°; C7···F5^{ii} 3.496 (3) Å, C7—H7···F5^{ii} 144 (2)°; C8···F2^{iii} 3.424 (3) Å, C8—H8··· F2^{iii} 127 (2)°; C17···F1^{iv} 3.571 (3) Å, C17—H17···F1^{iv} 163 (2)°. The shortest intermolecular contacts include: F4···F5^i 3.123 (2), F1···F5^{ii} 3.163 (2), F2···F4^{ii} 3.169 (2), F2···F5^{ii} 3.216 (2), C4···F5^i 3.199 (3) Å; symmetry codes: (i) $-x$, $\frac{1}{2} + y$, $\frac{1}{2} - z$; (ii) x, $y + 1$, z; (iii) x, $\frac{3}{2} - y$, $z - \frac{1}{2}$; (iv) x, $y - 1$, z.

Experimental

Single crystals were obtained by the slow evaporation of an ethanol solution of the compound.

Crystal data

$C_{18}H_{10}F_5P$	Mo $K\alpha$ radiation
$M_r = 352.23$	$\lambda = 0.71073$ Å
Monoclinic	Cell parameters from 37
$P2_1/c$	reflections
$a = 16.363 (2)$ Å	$\theta = 8-25°$
$b = 5.8964 (4)$ Å	$\mu = 0.225$ mm^{-1}
$c = 16.347 (1)$ Å	$T = 293 (2)$ K
$\beta = 96.84 (1)°$	Thin plate
$V = 1566.0 (2)$ Å^3	$0.60 \times 0.56 \times 0.12$ mm
$Z = 4$	Colourless
$D_x = 1.494$ Mg m^{-3}	
D_m not measured	

Data collection

Siemens $P4$ diffractometer	$\theta_{max} = 27.50°$
$\theta/2\theta$ scans	$h = -21 \rightarrow 21$
Absorption correction:	$k = -7 \rightarrow 1$
none	$l = -1 \rightarrow 21$
4711 measured reflections	3 standard reflections
3597 independent reflections	monitored every 97
2219 observed reflections	reflections
$[I > 2\sigma(I)]$	intensity decay: <3%
$R_{int} = 0.0234$	

Refinement

Refinement on F^2	$(\Delta/\sigma)_{max} < 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.0402$	$\Delta\rho_{max} = 0.28$ e Å^{-3}
$wR(F^2) = 0.1266$	$\Delta\rho_{min} = -0.26$ e Å^{-3}
$S = 0.921$	Extinction correction: none
3597 reflections	Atomic scattering factors
257 parameters	from *International Tables*
All H-atom parameters	*for Crystallography* (1992,
refined	Vol. C, Tables 4.2.6.8 and
$w = 1/[\sigma^2(F_o^2) + (0.0714P)^2]$	6.1.1.4)
where $P = (F_o^2 + 2F_c^2)/3$	

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
P	0.25943 (3)	0.00022 (10)	0.22166 (4)	0.0440 (2)
F1	0.24496 (8)	0.4497 (2)	0.32966 (9)	0.0598 (4)
F2	0.13126 (10)	0.5438 (3)	0.42738 (10)	0.0773 (5)
F3	0.00288 (10)	0.2571 (4)	0.43702 (11)	0.0948 (6)
F4	-0.00907 (9)	-0.1291 (3)	0.34582 (13)	0.0908 (6)
F5	0.10384 (8)	-0.2282 (2)	0.24751 (11)	0.0692 (4)
C1	0.18323 (12)	0.3005 (4)	0.33195 (13)	0.0443 (5)
C2	0.12482 (14)	0.3531 (4)	0.38222 (14)	0.0520 (6)
C3	0.05999 (14)	0.2083 (5)	0.3873 (2)	0.0598 (7)
C4	0.05427 (13)	0.0141 (5)	0.3418 (2)	0.0577 (6)
C5	0.11307 (13)	-0.0343 (4)	0.29183 (14)	0.0487 (5)
C6	0.18076 (12)	0.1037 (4)	0.28469 (13)	0.0407 (5)
C7	0.2057 (2)	0.3973 (5)	0.12832 (15)	0.0548 (6)
C8	0.2081 (2)	0.5412 (5)	0.0616 (2)	0.0634 (7)
C9	0.2609 (2)	0.4971 (5)	0.0042 (2)	0.0617 (7)
C10	0.3106 (2)	0.3094 (6)	0.0124 (2)	0.0647 (7)
C11	0.30798 (15)	0.1641 (5)	0.0781 (2)	0.0570 (6)
C12	0.25643 (12)	0.2080 (4)	0.13843 (13)	0.0437 (5)
C13	0.40023 (13)	0.2712 (4)	0.27868 (15)	0.0480 (5)
C14	0.47646 (14)	0.3004 (5)	0.3251 (2)	0.0555 (6)
C15	0.50843 (15)	0.1333 (5)	0.3782 (2)	0.0582 (7)
C16	0.4657 (2)	-0.0645 (5)	0.3852 (2)	0.0588 (7)
C17	0.39004 (14)	-0.0961 (4)	0.33822 (15)	0.0500 (6)
C18	0.35635 (12)	0.0718 (4)	0.28541 (12)	0.0406 (5)

Table 2. *Selected geometric parameters (Å, °)*

P—C12	1.827 (2)	F5—C5	1.353 (3)
P—C18	1.840 (2)	C1—C2	1.368 (3)
P—C6	1.846 (2)	C1—C6	1.392 (3)
F1—C1	1.343 (2)	C2—C3	1.372 (3)
F2—C2	1.342 (3)	C3—C4	1.363 (4)
F3—C3	1.341 (3)	C4—C5	1.364 (3)
F4—C4	1.345 (3)	C5 C6	1.391 (3)
C12—P—C18	102.29 (9)	F4—C4—C5	120.1 (2)
C12—P—C6	103.60 (10)	C3—C4—C5	119.7 (2)
C18—P—C6	102.67 (9)	F5—C5—C4	117.1 (2)
F1—C1—C2	116.7 (2)	F5—C5—C6	119.3 (2)
F1—C1—C6	120.2 (2)	C4—C5—C6	123.6 (2)
C2—C1—C6	123.1 (2)	C5—C6—C1	114.3 (2)
F2—C2—C1	120.4 (2)	C5—C6—P	118.0 (2)
F2—C2—C3	119.9 (2)	C1—C6—P	127.5 (2)
C1—C2—C3	119.7 (2)	C7—C12—P	126.2 (2)
F3—C3—C4	120.3 (2)	C11—C12—P	115.9 (2)
F3—C3—C2	120.2 (3)	C17—C18—P	116.2 (2)
C4—C3—C2	119.5 (2)	C13—C18 P	124.6 (2)
F4—C4—C3	120.3 (2)		

Data collection: *XSCANS* (Siemens, 1994). Cell refinement: *XSCANS*. Data reduction: *XSCANS*. Program used to solve structure: *SHELXTL/PC* (Sheldrick, 1990). Program used to refine structure: *SHELXL93* (Sheldrick, 1993). Geometrical calculations: *PARST* (Nardelli, 1983). Molecular graphics: *SHELXTL/PC*. Software used to prepare material for publication: *SHELXL93*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: MU1247). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

References

Daly, J. J. (1964). *J. Chem. Soc. A*, pp. 3799–3810.
Dunne, B. J. & Orpen, A. G. (1991). *Acta Cryst.* C47, 345–347.
Faggiani, R., Hao, N., Lock, C. J. L., Sayer, B. G. & McGlinchey, M. J. (1983). *Organometallics*, 2, 96–100.
Nardelli, M. (1983). *Comput. Chem.* 7, 95–98.
Orpen, A. G., Brammer, L., Allen, F. H., Kennard, O., Watson, D. G. & Taylor, R. (1989). *J. Chem. Soc. Dalton Trans.* pp. S1–83.
Shawkataly, O. B., Sivakumar, K. & Fun, H. K. (1996). In preparation.
Sheldrick, G. M. (1990). *SHELXTL/PC User's Manual*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1993). *SHELXL93. Program for Crystal Structure Refinement*. University of Göttingen, Germany.
Siemens (1994). *XSCANS User's Manual*. Version 2.1. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Papaefthymiou, 1984) and tri- or tetradentate bridging modes (Schake, Schmitt, Conti, Streib, Huffman, Hendrickson & Christou, 1991; Goldberg, Caneschi & Lippard, 1993). In an attempt to prepare lanthanoid(III) complexes containing 2,2′-biphenol or 2,2′-biphenoxide ligands, we obtained the title compound, (I).

(I)

All bond lengths and angles in (I) are comparable to related values reported in the literature (Allen *et al.*, 1987). The C(6)—C(7) bond between the two aromatic rings is significantly longer [1.491 (3) Å] than the C—C bonds within each ring. This is in agreement with the fact that, similar to the 2,2′-biphenoxide ligands in their metal complexes, the two aromatic rings in 2,2′-biphenol are not coplanar, but have a dihedral angle of 67.6 (1)° between them. It is noteworthy that the hydroxyl groups are *trans* with respect to one another, which is different to the *cis* relationship found for the 2,2′-biphenoxide ligand in its metal complexes (Schake *et al.*, 1991; Goldberg, Caneschi & Lippard,

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2,2′-Biphenol Monohydrate

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Abstract

The structure of the title compound (2,2′-biphenyldiol monohydrate, $C_{12}H_{10}O_2 \cdot H_2O$) is stabilized by hydrogen bonds between the lattice water molecules and the 2,2′-biphenol molecules, resulting in two-dimensional networks.

Comment

2,2′-Biphenol has attracted interest recently with regard to the synthesis of polynuclear transition metal complexes. 2,2′-Biphenoxide acts in both bidentate chelate (Coucouvanis, Salifoglou, Kanatzidis, Simopoulos &
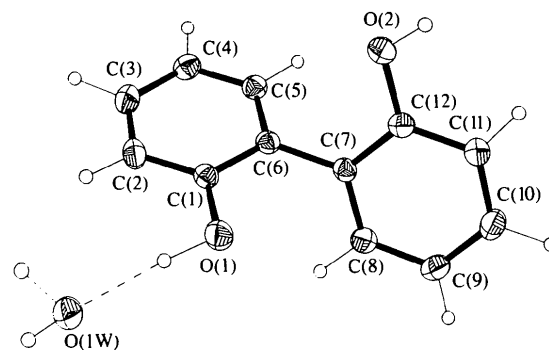

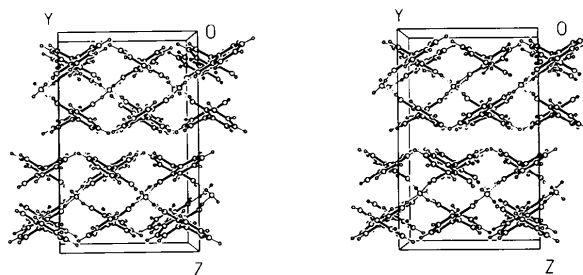Fig. 1. The structure of 2,2′-biphenol monohydrate showing 30% probability displacement ellipsoids.

Fig. 2. The molecular packing showing the hydrogen bonding in the crystal lattice.