Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

An orthorhombic polymorph of dichlorotris(pentafluorophenyl)phosphorane

Nicholas A. Barnes, Stephen M. Godfrey,* Ruth T. A. Halton, Imrana Mushtaq and Robin G. Pritchard

School of Chemistry, The University of Manchester (North Campus), Manchester M60 1QD, England

Correspondence e-mail: stephen.m.godfrey@manchester.ac.uk

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.039
wR factor = 0.101
Data-to-parameter ratio = 10.6

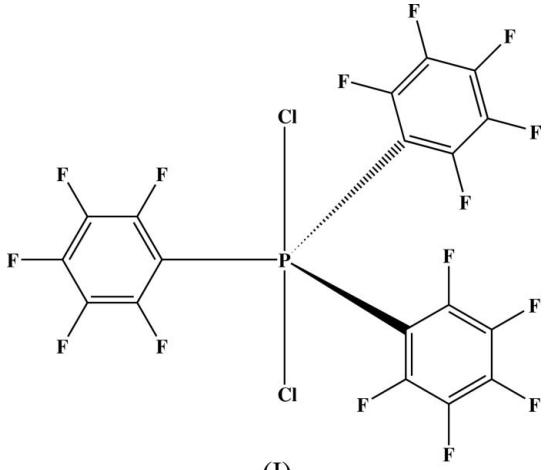
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

An orthorhombic form of dichlorotris(pentafluorophenyl)-phosphorane, $C_{18}Cl_2F_{15}P$, has been obtained as the product of the reaction between PhSeCl and $(C_6F_5)_3P$, and is a polymorph of the previously reported monoclinic form obtained from the reaction of $(C_6F_5)_3P$ with Cl_2. The molecule displays nearly perfect trigonal–bipyramidal geometry, and features a number of intermolecular F···F contacts, which lead to fluorous domains in the crystal packing.

Received 5 June 2006
Accepted 8 June 2006

Comment

Compounds of formula R_3PCl_2 are usually ionic in the solid state (Dillon *et al.*, 1976; Godfrey *et al.*, 1996, 1997; Ruthe *et al.*, 1997) and solution (Beveridge *et al.*, 1966; Wiley & Stine, 1967; Harris & Ali, 1968; Godfrey *et al.*, 1997); however, molecular five-coordinate trigonal–bipyramidal structures have been observed for R_3 = Ph_3, $(C_6F_5)Ph_2$ and $(C_6F_5)_3$ (Godfrey *et al.*, 1997; Godfrey, McAuliffe, Pritchard & Sheffield, 1998). Whilst the trigonal–bipyramidal form of Ph_3PCl_2 ionizes in solution, the analogous compounds containing highly electron withdrawing C_6F_5 groups retain their trigonal–bipyramidal geometry in solution. We have previously described the structure of the monoclinic form of $(C_6F_5)_3PCl_2$ (space group $P2_1/c$), prepared from $(C_6F_5)_3P$ and dichlorine (Godfrey *et al.*, 1997). We now report that the same compound is also formed when phenylselenenyl chloride is reacted with $(C_6F_5)_3P$; however the crystals obtained were an orthorhombic polymorph of $(C_6F_5)_3PCl_2$, (I) (see Fig. 1 and Table 1).



(I)

Compound (I) displays nearly perfect trigonal–bipyramidal geometry, although neither of the two polymorphs of $(C_6F_5)_3PCl_2$ display crystallographically imposed D_3

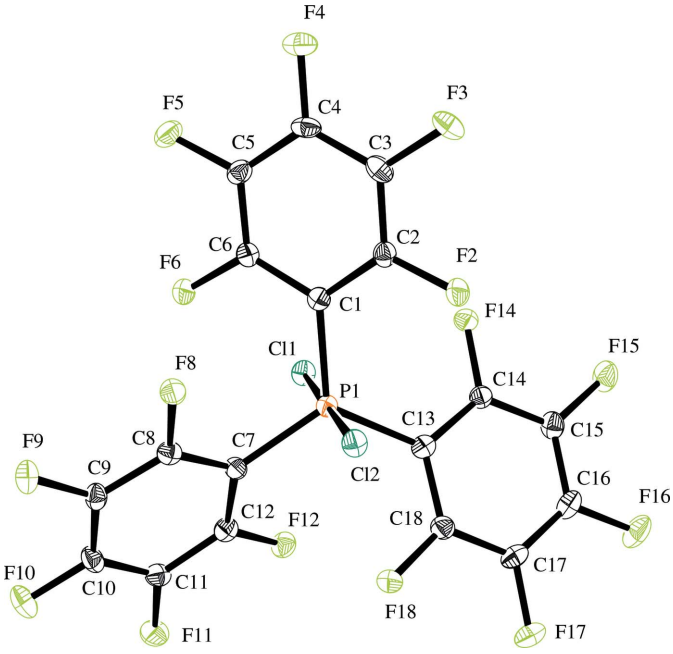


Figure 1
The structure of (I). Displacement ellipsoids are shown at the 30% probability level.

symmetry, unlike the analogous trigonal–bipyramidal $(C_6F_5)_3PBr_2$, space group $R\overline{3}c$ (Godfrey, McAuliffe, Mushtaq *et al.*, 1998). The P—Cl bonds in (I) are nearly equivalent and slightly shorter than observed in the monoclinic polymorph [P—Cl = 2.211 (2) Å; Godfrey *et al.*, 1997]. However, the P—Cl bonds are rather shorter than observed for $(C_6F_5)Ph_2PCl_2$ [P—Cl = 2.244 (2) and 2.241 (3) Å; Godfrey *et al.*, 1997] and Ph_3PCl_2 [P—Cl = 2.225 (1)–2.280 (2) Å; Godfrey, McAuliffe, Pritchard & Sheffield, 1998), reflecting the increased net electron-withdrawing capability of three C_6F_5 groups. The Cl—P—Cl angle is essentially linear, and the remaining angles around the P atom are close to ideal trigonal–bipyramidal geometry. The C—F bonds in the molecule vary in distance between 1.329 (3) and 1.349 (3) Å, with the C—F bonds to the *para*-F atoms being the shortest in each C_6F_5 group. A number of intermolecular F···F interactions, shorter than the sum of the van der Waals radii of two F atoms, (2.94 Å), are observed, which vary in length between 2.700 (2) Å and 2.900 (2) Å. The extended structure thus features extensive aggregation of the fluorous domains.

Experimental

The title compound was prepared by addition of $(C_6F_5)_3P$ (Aldrich) (0.273 g, 5.0×10^{-4} mol) to a freshly distilled diethyl ether solution (50 ml) containing PhSeCl (Aldrich) (0.196 g, 1.0×10^{-3} mol). The colour of the solution gradually changed from orange to yellow over several days. The solvent was reduced in volume to 10 ml, and colourless crystals of (I) formed at 273 K over several weeks. The spectroscopic data of (I) match the literature values (Godfrey *et al.*, 1997).

Crystal data

$C_{18}Cl_2F_{15}P$
M_r = 603.05
Orthorhombic, *Pbca*
a = 16.7367 (5) Å
b = 11.3713 (2) Å
c = 19.9214 (5) Å
V = 3791.40 (16) Å^3
Z = 8
D_x = 2.113 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.58 mm^{-1}
T = 150 (2) K
Prism, colourless
0.2 × 0.15 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.893, T_{max} = 0.944
19042 measured reflections
3458 independent reflections
2634 reflections with $I > 2\sigma(I)$
R_{int} = 0.071
θ_{max} = 25.3°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.101
S = 1.02
3458 reflections
325 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 3.0443P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.54 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—P1	1.820 (3)	P1—Cl2	2.1995 (10)
C7—P1	1.819 (3)	P1—Cl1	2.2005 (10)
C13—P1	1.821 (3)		
C7—P1—C1	118.64 (13)	C13—P1—Cl2	89.51 (9)
C7—P1—C13	121.49 (13)	C7—P1—Cl1	90.12 (9)
C1—P1—C13	119.86 (13)	C1—P1—Cl1	90.01 (9)
C7—P1—Cl2	90.26 (9)	C13—P1—Cl1	89.74 (9)
C1—P1—Cl2	90.37 (9)	Cl2—P1—Cl1	179.25 (5)

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We are grateful to the Engineering and Physical Sciences Research Council (EPSRC) for a research studentship to RTAH, and also for support of the UMIST X-ray facility (Research Initiative Grant).

References

Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
Beveridge, A. D., Harris, G. S. & Inglis, F. (1966). *J. Chem. Soc. A*, pp. 520–528.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Dillon, K. B., Lynch, R. J., Reeve, R. N. & Waddington, T. C. (1976). *J. Chem. Soc. Dalton Trans.* pp. 1243–1248.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Godfrey, S. M., McAuliffe, C. A., Mushtaq, I., Pritchard, R. G. & Sheffield, J. M. (1998). *J. Chem. Soc. Dalton Trans.* pp. 3815–3818.
Godfrey, S. M., McAuliffe, C. A., Pritchard, R. G. & Sheffield, J. M. (1996). *Chem. Commun.* pp. 2521–2522.
Godfrey, S. M., McAuliffe, C. A., Pritchard, R. G. & Sheffield, J. M. (1998). *Chem. Commun.* pp. 921–922.
Godfrey, S. M., McAuliffe, C. A., Pritchard, R. G., Sheffield, J. M. & Thompson, G. M. (1997). *J. Chem. Soc. Dalton Trans.* pp. 4823–4827.

Harris, G. S. & Ali, M. F. (1968). *Tetrahedron Lett.* **9**, 37–38.
Nonius (2000). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology,* Vol. 276, *Macromolecular Crystallography,* Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York, Academic Press.
Ruthe, F., du Mont, W.-W. & Jones, P. G. (1997). *Chem. Commun.* pp. 1947–1948.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Wiley, G. A. & Stine, W. R. (1967). *Tetrahedron Lett.* **8**, 2321–2324.

supporting information

Acta Cryst. (2006). E**62**, o2872–o2874 [https://doi.org/10.1107/S1600536806021751]

An orthorhombic polymorph of dichlorotris(pentafluorophenyl)phosphorane

Nicholas A. Barnes, Stephen M. Godfrey, Ruth T. A. Halton, Imrana Mushtaq and Robin G. Pritchard

dichlorotris(pentafluorophenyl)phosphorane

Crystal data

$C_{18}Cl_2F_{15}P$
$M_r = 603.05$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 16.7367$ (5) Å
$b = 11.3713$ (2) Å
$c = 19.9214$ (5) Å
$V = 3791.40$ (16) Å^3
$Z = 8$
$F(000) = 2336$
$D_x = 2.113$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 10582 reflections
$\theta = 1.0$–$25.4°$
$\mu = 0.58$ mm^{-1}
$T = 150$ K
Prism, colourless
0.2 × 0.15 × 0.1 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: Enraf Nonius FR590
Graphite monochromator
Detector resolution: 9 pixels mm^{-1}
φ or ω scans?
Absorption correction: multi-scan (Blessing, 1995)
$T_{min} = 0.893$, $T_{max} = 0.944$
19042 measured reflections
3458 independent reflections
2634 reflections with $I > 2\sigma(I)$
$R_{int} = 0.071$
$\theta_{max} = 25.3°$, $\theta_{min} = 3.0°$
$h = -20 \rightarrow 16$
$k = -13 \rightarrow 13$
$l = -23 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.101$
$S = 1.02$
3458 reflections
325 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 3.0443P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.54$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.49075 (17)	0.6096 (2)	0.37260 (13)	0.0238 (6)
C2	0.55870 (17)	0.5387 (2)	0.37278 (14)	0.0260 (6)
C3	0.55340 (19)	0.4188 (3)	0.37960 (14)	0.0299 (7)
C4	0.48042 (19)	0.3638 (2)	0.38180 (13)	0.0292 (7)
C5	0.41183 (18)	0.4310 (2)	0.37903 (14)	0.0286 (7)
C6	0.41747 (17)	0.5513 (2)	0.37650 (14)	0.0258 (6)
C7	0.41500 (17)	0.8501 (2)	0.33031 (14)	0.0247 (6)
C8	0.37070 (17)	0.7999 (2)	0.27868 (13)	0.0258 (6)
C9	0.30550 (17)	0.8560 (2)	0.25108 (13)	0.0270 (6)
C10	0.28672 (18)	0.9685 (3)	0.27131 (15)	0.0303 (7)
C11	0.33072 (18)	1.0219 (2)	0.32053 (15)	0.0290 (7)
C12	0.39230 (18)	0.9622 (2)	0.35101 (14)	0.0277 (6)
C13	0.58145 (17)	0.8449 (2)	0.40678 (14)	0.0262 (6)
C14	0.62486 (17)	0.7936 (2)	0.45900 (13)	0.0254 (6)
C15	0.69123 (19)	0.8466 (3)	0.48534 (14)	0.0308 (7)
C16	0.71409 (18)	0.9565 (3)	0.46304 (15)	0.0333 (7)
C17	0.67161 (19)	1.0105 (2)	0.41272 (15)	0.0307 (7)
C18	0.60700 (18)	0.9538 (2)	0.38398 (14)	0.0280 (6)
F2	0.63189 (10)	0.58597 (14)	0.36801 (8)	0.0314 (4)
F3	0.62094 (11)	0.35433 (14)	0.38288 (8)	0.0384 (4)
F4	0.47576 (12)	0.24731 (14)	0.38598 (8)	0.0389 (5)
F5	0.33989 (11)	0.37926 (14)	0.37902 (9)	0.0381 (4)
F6	0.34878 (10)	0.61209 (14)	0.37595 (8)	0.0310 (4)
F8	0.38919 (10)	0.69310 (13)	0.25486 (8)	0.0298 (4)
F9	0.26056 (10)	0.80222 (16)	0.20460 (8)	0.0367 (4)
F10	0.22484 (11)	1.02353 (16)	0.24344 (9)	0.0443 (5)
F11	0.31355 (11)	1.13189 (13)	0.33964 (9)	0.0398 (4)
F12	0.43149 (10)	1.01566 (14)	0.40148 (8)	0.0327 (4)
F14	0.60279 (10)	0.68909 (13)	0.48410 (8)	0.0296 (4)
F15	0.73410 (11)	0.79176 (17)	0.53271 (8)	0.0426 (5)
F16	0.77747 (12)	1.00955 (17)	0.49033 (9)	0.0480 (5)
F17	0.69268 (12)	1.11803 (14)	0.39190 (9)	0.0415 (5)
F18	0.56887 (10)	1.00802 (14)	0.33355 (9)	0.0342 (4)
P1	0.49612 (4)	0.76936 (6)	0.36995 (3)	0.02308 (18)
Cl1	0.43366 (4)	0.77888 (6)	0.46700 (3)	0.02886 (19)
Cl2	0.55989 (4)	0.76107 (6)	0.27353 (3)	0.02870 (19)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0251 (16)	0.0259 (14)	0.0204 (13)	−0.0007 (11)	0.0001 (11)	0.0002 (11)
C2	0.0227 (16)	0.0316 (15)	0.0238 (14)	−0.0006 (12)	0.0013 (11)	0.0023 (12)
C3	0.0336 (18)	0.0323 (15)	0.0237 (14)	0.0099 (13)	0.0007 (12)	0.0003 (12)
C4	0.046 (2)	0.0198 (13)	0.0220 (14)	−0.0004 (13)	−0.0044 (13)	0.0037 (11)
C5	0.0314 (17)	0.0295 (14)	0.0250 (14)	−0.0077 (13)	−0.0021 (12)	0.0039 (12)
C6	0.0247 (16)	0.0280 (14)	0.0246 (14)	0.0011 (12)	−0.0009 (11)	0.0001 (12)
C7	0.0231 (15)	0.0249 (13)	0.0261 (14)	0.0012 (11)	−0.0001 (12)	0.0030 (12)
C8	0.0263 (16)	0.0266 (14)	0.0245 (14)	0.0003 (12)	0.0035 (12)	0.0013 (12)
C9	0.0208 (15)	0.0369 (15)	0.0234 (14)	−0.0012 (12)	0.0003 (12)	0.0021 (12)
C10	0.0218 (16)	0.0377 (16)	0.0314 (16)	0.0071 (13)	0.0010 (13)	0.0069 (13)
C11	0.0257 (16)	0.0245 (14)	0.0367 (17)	0.0046 (12)	0.0086 (13)	0.0016 (12)
C12	0.0279 (16)	0.0296 (14)	0.0255 (14)	−0.0026 (12)	0.0018 (12)	−0.0009 (12)
C13	0.0274 (16)	0.0257 (14)	0.0256 (14)	−0.0014 (12)	0.0030 (12)	−0.0020 (12)
C14	0.0246 (16)	0.0282 (14)	0.0232 (14)	−0.0010 (12)	0.0027 (11)	0.0029 (12)
C15	0.0295 (17)	0.0419 (17)	0.0211 (14)	−0.0017 (14)	−0.0034 (12)	0.0017 (13)
C16	0.0295 (18)	0.0401 (17)	0.0302 (16)	−0.0113 (14)	0.0029 (13)	−0.0053 (14)
C17	0.0333 (18)	0.0278 (14)	0.0311 (15)	−0.0078 (13)	0.0085 (13)	−0.0013 (13)
C18	0.0273 (16)	0.0284 (14)	0.0284 (15)	0.0007 (12)	0.0020 (13)	0.0029 (12)
F2	0.0227 (9)	0.0351 (9)	0.0363 (9)	0.0026 (7)	0.0013 (7)	0.0007 (7)
F3	0.0419 (11)	0.0343 (9)	0.0388 (10)	0.0170 (8)	0.0028 (8)	0.0027 (8)
F4	0.0597 (13)	0.0233 (8)	0.0337 (9)	−0.0009 (8)	−0.0043 (8)	0.0011 (7)
F5	0.0383 (11)	0.0357 (9)	0.0401 (10)	−0.0148 (8)	−0.0026 (8)	0.0054 (8)
F6	0.0230 (9)	0.0333 (9)	0.0366 (9)	−0.0008 (7)	−0.0003 (7)	0.0028 (7)
F8	0.0306 (9)	0.0268 (8)	0.0320 (9)	0.0021 (7)	−0.0031 (7)	−0.0046 (7)
F9	0.0268 (10)	0.0485 (10)	0.0349 (9)	−0.0004 (8)	−0.0066 (8)	−0.0040 (8)
F10	0.0348 (11)	0.0503 (11)	0.0479 (11)	0.0174 (9)	−0.0072 (9)	0.0041 (9)
F11	0.0371 (11)	0.0273 (8)	0.0551 (11)	0.0096 (8)	0.0035 (9)	−0.0028 (8)
F12	0.0322 (10)	0.0288 (8)	0.0370 (10)	−0.0019 (7)	−0.0023 (8)	−0.0069 (7)
F14	0.0314 (10)	0.0284 (8)	0.0290 (8)	−0.0020 (7)	−0.0035 (7)	0.0061 (7)
F15	0.0368 (11)	0.0582 (12)	0.0329 (9)	−0.0098 (9)	−0.0121 (8)	0.0083 (9)
F16	0.0436 (12)	0.0586 (12)	0.0417 (10)	−0.0262 (10)	−0.0081 (9)	−0.0027 (9)
F17	0.0451 (12)	0.0301 (9)	0.0494 (11)	−0.0130 (8)	0.0052 (9)	0.0013 (8)
F18	0.0318 (10)	0.0307 (9)	0.0402 (10)	−0.0011 (7)	−0.0017 (8)	0.0103 (8)
P1	0.0218 (4)	0.0236 (4)	0.0238 (4)	−0.0005 (3)	−0.0001 (3)	0.0009 (3)
Cl1	0.0278 (4)	0.0336 (4)	0.0251 (4)	−0.0002 (3)	0.0038 (3)	−0.0011 (3)
Cl2	0.0264 (4)	0.0358 (4)	0.0239 (3)	0.0008 (3)	0.0031 (3)	0.0018 (3)

Geometric parameters (Å, º)

C1—C2	1.394 (4)	C10—F10	1.332 (3)
C1—C6	1.396 (4)	C10—C11	1.368 (4)
C1—P1	1.820 (3)	C11—F11	1.339 (3)
C2—F2	1.341 (3)	C11—C12	1.375 (4)
C2—C3	1.373 (4)	C12—F12	1.346 (3)
C3—F3	1.349 (3)	C13—C18	1.387 (4)

C3—C4	1.373 (4)	C13—C14	1.396 (4)
C4—F4	1.329 (3)	C13—P1	1.821 (3)
C4—C5	1.381 (4)	C14—F14	1.342 (3)
C5—F5	1.340 (3)	C14—C15	1.368 (4)
C5—C6	1.372 (4)	C15—F15	1.340 (3)
C6—F6	1.341 (3)	C15—C16	1.381 (4)
C7—C8	1.390 (4)	C16—F16	1.336 (3)
C7—C12	1.393 (4)	C16—C17	1.374 (4)
C7—P1	1.819 (3)	C17—F17	1.339 (3)
C8—F8	1.340 (3)	C17—C18	1.383 (4)
C8—C9	1.379 (4)	C18—F18	1.340 (3)
C9—F9	1.341 (3)	P1—Cl2	2.1995 (10)
C9—C10	1.377 (4)	P1—Cl1	2.2005 (10)
C2—C1—C6	116.3 (3)	C10—C11—C12	120.0 (2)
C2—C1—P1	122.5 (2)	F12—C12—C11	118.2 (2)
C6—C1—P1	121.2 (2)	F12—C12—C7	120.1 (3)
F2—C2—C3	117.6 (3)	C11—C12—C7	121.7 (3)
F2—C2—C1	120.9 (2)	C18—C13—C14	117.1 (3)
C3—C2—C1	121.4 (3)	C18—C13—P1	122.1 (2)
F3—C3—C2	119.4 (3)	C14—C13—P1	120.8 (2)
F3—C3—C4	119.7 (3)	F14—C14—C15	118.1 (2)
C2—C3—C4	120.9 (3)	F14—C14—C13	120.3 (2)
F4—C4—C3	120.6 (3)	C15—C14—C13	121.6 (3)
F4—C4—C5	120.4 (3)	F15—C15—C14	120.0 (3)
C3—C4—C5	119.1 (3)	F15—C15—C16	120.0 (3)
F5—C5—C6	120.0 (3)	C14—C15—C16	120.0 (3)
F5—C5—C4	120.2 (2)	F16—C16—C17	120.4 (3)
C6—C5—C4	119.8 (3)	F16—C16—C15	119.9 (3)
F6—C6—C5	117.1 (3)	C17—C16—C15	119.7 (3)
F6—C6—C1	120.5 (2)	F17—C17—C16	119.8 (3)
C5—C6—C1	122.4 (3)	F17—C17—C18	120.2 (3)
C8—C7—C12	116.7 (3)	C16—C17—C18	119.9 (3)
C8—C7—P1	120.8 (2)	F18—C18—C17	117.9 (2)
C12—C7—P1	122.5 (2)	F18—C18—C13	120.6 (3)
F8—C8—C9	117.5 (2)	C17—C18—C13	121.4 (3)
F8—C8—C7	120.7 (3)	C7—P1—C1	118.64 (13)
C9—C8—C7	121.8 (3)	C7—P1—C13	121.49 (13)
F9—C9—C10	119.9 (3)	C1—P1—C13	119.86 (13)
F9—C9—C8	120.6 (2)	C7—P1—Cl2	90.26 (9)
C10—C9—C8	119.6 (3)	C1—P1—Cl2	90.37 (9)
F10—C10—C11	120.6 (3)	C13—P1—Cl2	89.51 (9)
F10—C10—C9	119.5 (3)	C7—P1—Cl1	90.12 (9)
C11—C10—C9	119.9 (3)	C1—P1—Cl1	90.01 (9)
F11—C11—C10	120.2 (3)	C13—P1—Cl1	89.74 (9)
F11—C11—C12	119.8 (3)	Cl2—P1—Cl1	179.25 (5)
C6—C1—C2—F2	178.8 (2)	C18—C13—C14—F14	179.1 (2)

P1—C1—C2—F2	−2.9 (4)	P1—C13—C14—F14	−1.9 (4)
C6—C1—C2—C3	−2.9 (4)	C18—C13—C14—C15	−1.9 (4)
P1—C1—C2—C3	175.3 (2)	P1—C13—C14—C15	177.1 (2)
F2—C2—C3—F3	1.6 (4)	F14—C14—C15—F15	2.9 (4)
C1—C2—C3—F3	−176.7 (2)	C13—C14—C15—F15	−176.1 (3)
F2—C2—C3—C4	−177.1 (3)	F14—C14—C15—C16	−177.2 (3)
C1—C2—C3—C4	4.6 (4)	C13—C14—C15—C16	3.8 (4)
F3—C3—C4—F4	−1.2 (4)	F15—C15—C16—F16	−2.2 (4)
C2—C3—C4—F4	177.6 (2)	C14—C15—C16—F16	177.9 (3)
F3—C3—C4—C5	179.4 (2)	F15—C15—C16—C17	177.6 (3)
C2—C3—C4—C5	−1.9 (4)	C14—C15—C16—C17	−2.3 (4)
F4—C4—C5—F5	−1.5 (4)	F16—C16—C17—F17	−1.5 (4)
C3—C4—C5—F5	178.0 (3)	C15—C16—C17—F17	178.7 (3)
F4—C4—C5—C6	178.3 (2)	F16—C16—C17—C18	178.8 (3)
C3—C4—C5—C6	−2.3 (4)	C15—C16—C17—C18	−1.0 (4)
F5—C5—C6—F6	1.8 (4)	F17—C17—C18—F18	2.5 (4)
C4—C5—C6—F6	−178.0 (2)	C16—C17—C18—F18	−177.9 (3)
F5—C5—C6—C1	−176.3 (3)	F17—C17—C18—C13	−176.8 (3)
C4—C5—C6—C1	3.9 (4)	C16—C17—C18—C13	2.9 (4)
C2—C1—C6—F6	−179.3 (2)	C14—C13—C18—F18	179.3 (2)
P1—C1—C6—F6	2.4 (4)	P1—C13—C18—F18	0.3 (4)
C2—C1—C6—C5	−1.3 (4)	C14—C13—C18—C17	−1.4 (4)
P1—C1—C6—C5	−179.5 (2)	P1—C13—C18—C17	179.6 (2)
C12—C7—C8—F8	178.9 (2)	C8—C7—P1—C1	−28.9 (3)
P1—C7—C8—F8	−3.1 (4)	C12—C7—P1—C1	149.0 (2)
C12—C7—C8—C9	−2.6 (4)	C8—C7—P1—C13	151.3 (2)
P1—C7—C8—C9	175.4 (2)	C12—C7—P1—C13	−30.9 (3)
F8—C8—C9—F9	3.2 (4)	C8—C7—P1—Cl2	61.7 (2)
C7—C8—C9—F9	−175.4 (2)	C12—C7—P1—Cl2	−120.5 (2)
F8—C8—C9—C10	−176.5 (2)	C8—C7—P1—Cl1	−118.9 (2)
C7—C8—C9—C10	4.9 (4)	C12—C7—P1—Cl1	58.9 (2)
F9—C9—C10—F10	−1.3 (4)	C2—C1—P1—C7	150.5 (2)
C8—C9—C10—F10	178.4 (2)	C6—C1—P1—C7	−31.3 (3)
F9—C9—C10—C11	177.6 (3)	C2—C1—P1—C13	−29.7 (3)
C8—C9—C10—C11	−2.7 (4)	C6—C1—P1—C13	148.5 (2)
F10—C10—C11—F11	−2.2 (4)	C2—C1—P1—Cl2	60.0 (2)
C9—C10—C11—F11	178.9 (2)	C6—C1—P1—Cl2	−121.9 (2)
F10—C10—C11—C12	177.1 (3)	C2—C1—P1—Cl1	−119.4 (2)
C9—C10—C11—C12	−1.7 (4)	C6—C1—P1—Cl1	58.8 (2)
F11—C11—C12—F12	2.7 (4)	C18—C13—P1—C7	−27.6 (3)
C10—C11—C12—F12	−176.7 (3)	C14—C13—P1—C7	153.4 (2)
F11—C11—C12—C7	−176.5 (3)	C18—C13—P1—C1	152.5 (2)
C10—C11—C12—C7	4.1 (4)	C14—C13—P1—C1	−26.4 (3)
C8—C7—C12—F12	178.9 (2)	C18—C13—P1—Cl2	62.4 (2)
P1—C7—C12—F12	1.0 (4)	C14—C13—P1—Cl2	−116.6 (2)
C8—C7—C12—C11	−2.0 (4)	C18—C13—P1—Cl1	−117.6 (2)
P1—C7—C12—C11	−179.9 (2)	C14—C13—P1—Cl1	63.4 (2)