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(*R*)-2,2′-Bis(diphenylphosphino)-6,6′-bis(tridecafluoro-*n*-hexyl)-1,1′-binaphthyl

John Fawcett,* Eric G. Hope, Alison M. Stuart and Andrew J. West

Department of Chemistry, University of Leicester, Leicester LE1 7RH, England

Correspondence e-mail: jxf@leicester.ac.uk

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.058
wR factor = 0.174
Data-to-parameter ratio = 13.1

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

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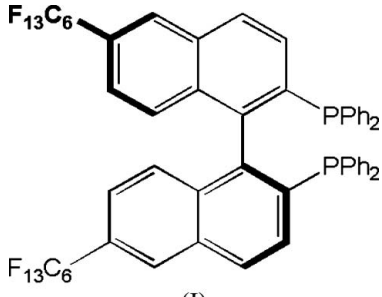
The molecule of the title compound, $C_{56}H_{30}F_{26}P_2$, is located on a twofold axis perpendicular to the central C—C bond of the binaphthyl group and the P atoms have the typical pseudo-tetrahedral geometry found for compounds of this type.

Comment

We have probed the application of perfluoroalkylated phosphorus(III) ligands for catalysis in perfluorocarbon solvents as alternative reaction media to conventional organic solvents (Stuart *et al.*, 2000; Foster, Adams *et al.*, 2002; Foster, Gudmunsen *et al.*, 2002), including structural characterizations of a number of perfluoroalkylated phosphine coordination compounds (Fawcett *et al.*, 1997, 1998, 2001). More recently, we turned our attention to asymmetric catalysis, including the synthesis of (*R*)-2,2′-bis(diphenylphosphino)-6,6′-bis(tridecafluoro-*n*-hexyl)-1,1′-binaphthyl and (*R*)-2,2′-bis(diphenylphosphino)-6,6′-bis(1*H*,1*H*,2*H*,2*H*-tridecafluorooctyl)-1,1′-binaphthyl, and their application in ruthenium-catalysed hydrogenation in methanol (Birdsall *et al.*, 2001) and dichloromethane with ligand recycling using fluorous silica gel (Hope *et al.*, 2004). Although we have previously structurally characterized perfluoroalkylated triphenylphosphine oxides (Bhattacharyya *et al.*, 2000; Croxtall *et al.*, 2002), there have been no previous single-crystal structure determinations of phosphine ligands with fluorous tails. We present here the crystal structure of the title such ligand, (I).



(I)

The molecular structure of (I), viewed down the C2—C2′ pivot (Fig. 1), clearly shows the non-coplanar geometry of the two naphthyl ring systems, in which the perfluoroalkyl chains adopt conformations in the solid state that minimize their interactions with each other. The molecule is located on a twofold axis perpendicular to the C2—C2′ bond of the binaphthyl group and the P atoms have the typical pseudo-tetrahedral geometry found for other structurally characterized BINAP complexes (Ozawa *et al.*, 1993). The P—C bond

distances are very similar to those found for metal-bound BINAP ligands, suggesting that any influence of the perfluoroalkyl unit does not manifest itself in the P—C(naphthyl) bond length. However, the C—P—C bond angles are all smaller [104.75 (13), 100.35 (12) and 103.01 (12)°, *cf.* 106.7 (5), 105.7 (4) and 105.1 (4)°], reflecting the stereochemical activity of the P lone pair.

The perfluoroalkyl unit is kinked (Fawcett *et al.*, 1998), with a single *gauche* conformation [C11—C12—C13—C14 −60.0 (4)°], as opposed to the more usual *trans* staggered conformation [C13—C14—C15—C16 167.7 (3)°] found for linear perfluoroalkyl chains.

Although within each individual molecule the perfluoroalkyl chains have no interactions, the molecular packing of (I) shows that the fluorinated groups and binaphthyl rings are stacked in alternate layers perpendicular to the *c* axis, to generate fluorous and hydrocarbon domains, characteristic of structural characterizations of fluorous materials (Fawcett *et al.*, 1997, 1998).

Experimental

The title compound was synthesized by the literature route of Birdsall *et al.* (2001). Crystals of (I) suitable for structural characterization were grown by slow evaporation of a solution of the compound in a diethyl ether–hexane (1:6) mixture.

Crystal data

$C_{56}H_{30}F_{26}P_2$
M_r = 1258.74
Monoclinic, $C2/c$
a = 19.456 (3) Å
b = 8.2838 (9) Å
c = 31.886 (4) Å
β = 101.212 (4)°
V = 5040.9 (11) Å^3
Z = 4
D_x = 1.659 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5639 reflections
θ = 2.3–25.4°
μ = 0.22 mm^{-1}
T = 150 (2) K
Block, colourless
0.34 × 0.16 × 0.14 mm

Data collection

Bruker APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.888, T_{max} = 0.982
19219 measured reflections
4947 independent reflections
4108 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 26.0°
$h = -23 \rightarrow 23$
$k = -10 \rightarrow 10$
$l = -39 \rightarrow 39$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.174
S = 1.03
4947 reflections
379 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1018P)^2 + 8.8615P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

A 2.6 e Å^{-3} residual electron-density peak located 1.3 Å from the unique P atom may be refined as a 20% occupancy O atom, due to partial oxidation to the phosphine oxide; by comparison, the electron density for a typical C atom is found to be 7.5 e Å^{-3}. For the final refinement, however, the site was assumed to be occupied by a lone pair, and subsequent calculations of formula weight, density and absorption coefficient are based on this model. All H atoms were included in calculated positions as riding atoms, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C).

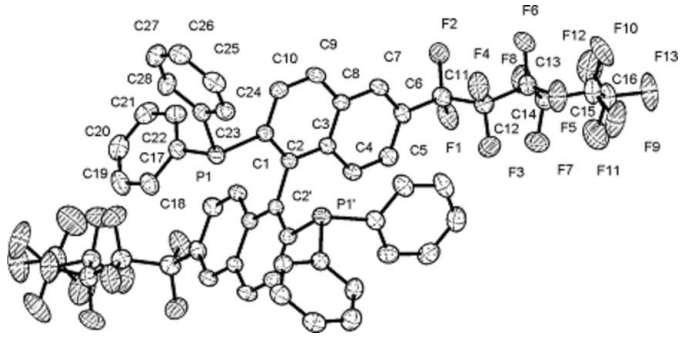


Figure 1
The molecular structure of (I), showing the atom-labelling scheme and with 50% probability displacement ellipsoids. H atoms have been omitted for clarity. The molecule is located on a twofold axis; primed atoms are generated by the symmetry operator $(1 - x, y, \frac{1}{2} - z)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

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$h = -23 \rightarrow 23$
$k = -10 \rightarrow 10$
$l = -39 \rightarrow 39$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.174$
$S = 1.03$
4947 reflections
379 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1018P)^2 + 8.8615P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 2.64$ e Å^{-3}
$\Delta\rho_{min} = -0.43$ e Å^{-3}

Special details

Experimental. absorption correction based on 8821 reflections (*SADABS*); R_{int} 0.030 and 0.020 before and after correction respectively.

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. The 2.6 e residual electron density peak at 1.3 Å from the P atom is assigned to a lone pair. The comparative electron density for a typical C atom is found to be 7.5 e. 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}
P1	0.45105 (4)	0.57171 (9)	0.19205 (2)	0.0240 (2)
C1	0.41698 (13)	0.7058 (3)	0.22869 (8)	0.0211 (5)
C2	0.46233 (13)	0.8151 (3)	0.25218 (8)	0.0192 (5)
C3	0.43890 (13)	0.9215 (3)	0.28082 (8)	0.0195 (5)
C4	0.48209 (14)	1.0392 (3)	0.30439 (9)	0.0232 (6)
H4	0.5294	1.0481	0.3011	0.028*
C5	0.45802 (14)	1.1402 (3)	0.33161 (9)	0.0260 (6)
H5	0.4882	1.2195	0.3469	0.031*
C6	0.38786 (14)	1.1279 (3)	0.33732 (9)	0.0245 (6)
C7	0.34482 (14)	1.0146 (3)	0.31547 (9)	0.0241 (6)
H7	0.2980	1.0056	0.3198	0.029*
C8	0.36832 (13)	0.9108 (3)	0.28668 (8)	0.0211 (5)
C9	0.32348 (14)	0.7968 (3)	0.26250 (9)	0.0262 (6)
H9	0.2762	0.7887	0.2660	0.031*
C10	0.34688 (14)	0.6986 (4)	0.23435 (9)	0.0257 (6)
H10	0.3156	0.6235	0.2181	0.031*
C11	0.36189 (15)	1.2390 (3)	0.36738 (10)	0.0280 (6)
C12	0.37201 (15)	1.1767 (3)	0.41326 (9)	0.0280 (6)
C13	0.34205 (16)	1.2728 (4)	0.44720 (10)	0.0313 (7)
C14	0.36787 (15)	1.4466 (4)	0.45705 (9)	0.0291 (6)
C15	0.35339 (19)	1.5150 (4)	0.49944 (10)	0.0381 (8)
C16	0.3643 (2)	1.6954 (4)	0.50526 (11)	0.0410 (8)
C17	0.44434 (15)	0.7024 (3)	0.14575 (9)	0.0256 (6)
C18	0.50054 (17)	0.7039 (4)	0.12490 (10)	0.0322 (7)
H18	0.5394	0.6345	0.1343	0.039*
C19	0.50046 (19)	0.8046 (4)	0.09083 (11)	0.0386 (8)
H19	0.5393	0.8051	0.0768	0.046*
C20	0.44476 (18)	0.9046 (4)	0.07683 (10)	0.0387 (8)
H20	0.4447	0.9733	0.0530	0.046*
C21	0.38885 (17)	0.9051 (4)	0.09745 (11)	0.0374 (7)
H21	0.3502	0.9749	0.0879	0.045*
C22	0.38890 (16)	0.8050 (4)	0.13172 (10)	0.0311 (7)
H22	0.3503	0.8065	0.1459	0.037*
C23	0.38094 (14)	0.4253 (3)	0.17720 (9)	0.0231 (6)
C24	0.37704 (15)	0.3049 (4)	0.20648 (10)	0.0289 (6)
H24	0.4075	0.3075	0.2337	0.035*
C25	0.32942 (16)	0.1809 (4)	0.19674 (10)	0.0325 (7)
H25	0.3273	0.0982	0.2171	0.039*

C26	0.28513 (16)	0.1766 (4)	0.15775 (10)	0.0326 (7)
H26	0.2520	0.0916	0.1511	0.039*
C27	0.28865 (17)	0.2951 (4)	0.12832 (10)	0.0339 (7)
H27	0.2581	0.2916	0.1012	0.041*
C28	0.33619 (16)	0.4194 (4)	0.13784 (9)	0.0296 (6)
H28	0.3382	0.5014	0.1173	0.036*
F1	0.39364 (11)	1.3829 (2)	0.36898 (6)	0.0424 (5)
F2	0.29221 (9)	1.2669 (2)	0.35441 (6)	0.0403 (5)
F3	0.44071 (10)	1.1583 (2)	0.42805 (6)	0.0420 (5)
F4	0.34198 (11)	1.0313 (2)	0.41220 (6)	0.0440 (5)
F5	0.35830 (13)	1.1881 (2)	0.48348 (6)	0.0487 (5)
F6	0.27245 (10)	1.2752 (3)	0.43570 (6)	0.0484 (5)
F7	0.43593 (9)	1.4547 (2)	0.45807 (7)	0.0445 (5)
F8	0.33550 (11)	1.5416 (2)	0.42554 (6)	0.0438 (5)
F9	0.39797 (15)	1.4458 (3)	0.53160 (7)	0.0681 (7)
F10	0.28870 (13)	1.4815 (3)	0.50290 (8)	0.0609 (7)
F11	0.42631 (14)	1.7400 (3)	0.49946 (8)	0.0670 (7)
F12	0.31807 (15)	1.7773 (3)	0.47828 (8)	0.0656 (7)
F13	0.35669 (16)	1.7377 (3)	0.54363 (7)	0.0662 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
P1	0.0243 (4)	0.0231 (4)	0.0253 (4)	−0.0001 (3)	0.0061 (3)	−0.0042 (3)
C1	0.0197 (13)	0.0218 (13)	0.0216 (13)	0.0019 (10)	0.0033 (10)	−0.0003 (10)
C2	0.0181 (13)	0.0206 (13)	0.0193 (12)	0.0008 (10)	0.0048 (10)	0.0042 (10)
C3	0.0196 (13)	0.0194 (13)	0.0200 (13)	0.0015 (10)	0.0046 (10)	0.0030 (10)
C4	0.0197 (13)	0.0243 (14)	0.0264 (14)	−0.0018 (10)	0.0063 (10)	0.0006 (11)
C5	0.0274 (14)	0.0219 (14)	0.0287 (15)	−0.0045 (11)	0.0058 (11)	−0.0037 (11)
C6	0.0285 (14)	0.0228 (14)	0.0239 (14)	0.0023 (11)	0.0093 (11)	−0.0007 (11)
C7	0.0199 (13)	0.0259 (14)	0.0276 (14)	0.0010 (11)	0.0078 (11)	0.0019 (11)
C8	0.0188 (13)	0.0235 (13)	0.0212 (13)	0.0015 (10)	0.0047 (10)	0.0021 (10)
C9	0.0179 (13)	0.0304 (15)	0.0316 (15)	−0.0023 (11)	0.0081 (11)	−0.0019 (12)
C10	0.0208 (13)	0.0282 (15)	0.0275 (14)	−0.0044 (11)	0.0031 (11)	−0.0049 (11)
C11	0.0293 (15)	0.0233 (14)	0.0326 (16)	0.0025 (12)	0.0087 (12)	−0.0029 (12)
C12	0.0293 (15)	0.0244 (14)	0.0301 (15)	0.0020 (12)	0.0055 (12)	−0.0035 (12)
C13	0.0331 (16)	0.0350 (17)	0.0266 (15)	0.0009 (13)	0.0078 (12)	−0.0014 (13)
C14	0.0307 (15)	0.0310 (16)	0.0267 (15)	0.0076 (12)	0.0084 (12)	−0.0010 (12)
C15	0.056 (2)	0.0342 (17)	0.0254 (16)	0.0073 (15)	0.0125 (14)	−0.0002 (13)
C16	0.056 (2)	0.0376 (18)	0.0319 (17)	0.0030 (16)	0.0152 (15)	−0.0067 (14)
C17	0.0281 (14)	0.0231 (14)	0.0263 (14)	−0.0054 (11)	0.0074 (11)	−0.0066 (11)
C18	0.0376 (17)	0.0272 (15)	0.0350 (16)	−0.0016 (13)	0.0151 (13)	−0.0074 (12)
C19	0.049 (2)	0.0359 (18)	0.0369 (18)	−0.0100 (15)	0.0225 (15)	−0.0068 (14)
C20	0.052 (2)	0.0325 (17)	0.0309 (16)	−0.0134 (15)	0.0062 (14)	0.0006 (13)
C21	0.0366 (17)	0.0329 (17)	0.0390 (18)	−0.0048 (13)	−0.0015 (13)	0.0058 (14)
C22	0.0263 (15)	0.0311 (16)	0.0354 (16)	−0.0034 (12)	0.0049 (12)	−0.0004 (13)
C23	0.0243 (14)	0.0210 (13)	0.0249 (14)	0.0030 (10)	0.0071 (11)	−0.0026 (11)
C24	0.0263 (15)	0.0313 (16)	0.0292 (15)	0.0048 (12)	0.0059 (12)	0.0031 (12)

C25	0.0339 (16)	0.0247 (15)	0.0412 (18)	0.0038 (12)	0.0129 (13)	0.0087 (13)
C26	0.0308 (16)	0.0243 (15)	0.0438 (18)	−0.0055 (12)	0.0102 (13)	−0.0061 (13)
C27	0.0387 (17)	0.0304 (16)	0.0303 (16)	−0.0052 (13)	0.0014 (13)	−0.0046 (13)
C28	0.0378 (16)	0.0252 (15)	0.0250 (14)	−0.0038 (12)	0.0039 (12)	−0.0011 (11)
F1	0.0653 (13)	0.0219 (9)	0.0476 (11)	−0.0067 (8)	0.0301 (10)	−0.0071 (8)
F2	0.0365 (10)	0.0485 (11)	0.0351 (10)	0.0199 (9)	0.0045 (8)	−0.0075 (8)
F3	0.0366 (10)	0.0436 (11)	0.0420 (11)	0.0166 (8)	−0.0019 (8)	−0.0116 (9)
F4	0.0686 (14)	0.0271 (10)	0.0399 (11)	−0.0099 (9)	0.0193 (10)	−0.0032 (8)
F5	0.0847 (16)	0.0350 (11)	0.0289 (10)	0.0026 (10)	0.0169 (10)	0.0041 (8)
F6	0.0321 (10)	0.0682 (14)	0.0490 (12)	−0.0091 (9)	0.0178 (9)	−0.0215 (10)
F7	0.0328 (10)	0.0432 (11)	0.0583 (13)	−0.0016 (8)	0.0112 (9)	−0.0201 (10)
F8	0.0659 (13)	0.0370 (10)	0.0278 (9)	0.0176 (9)	0.0075 (9)	0.0038 (8)
F9	0.120 (2)	0.0472 (13)	0.0295 (11)	0.0231 (13)	−0.0036 (12)	0.0006 (10)
F10	0.0740 (15)	0.0546 (14)	0.0694 (15)	−0.0159 (12)	0.0517 (13)	−0.0230 (12)
F11	0.0760 (17)	0.0554 (14)	0.0760 (17)	−0.0183 (12)	0.0310 (14)	−0.0301 (13)
F12	0.0995 (19)	0.0396 (12)	0.0552 (14)	0.0253 (12)	0.0087 (13)	−0.0023 (10)
F13	0.124 (2)	0.0431 (12)	0.0404 (12)	−0.0012 (13)	0.0384 (13)	−0.0145 (10)

Geometric parameters (Å, º)

P1—C17	1.815 (3)	C14—F8	1.334 (3)
P1—C23	1.818 (3)	C14—C15	1.541 (4)
P1—C1	1.827 (3)	C15—F10	1.314 (4)
C1—C2	1.379 (4)	C15—F9	1.337 (4)
C1—C10	1.411 (4)	C15—C16	1.516 (5)
C2—C3	1.408 (4)	C16—F12	1.307 (4)
C2—C2^{i}	1.499 (5)	C16—F13	1.308 (4)
C3—C4	1.406 (4)	C16—F11	1.309 (4)
C3—C8	1.424 (4)	C17—C22	1.378 (4)
C4—C5	1.353 (4)	C17—C18	1.386 (4)
C4—H4	0.950	C18—C19	1.369 (5)
C5—C6	1.416 (4)	C18—H18	0.950
C5—H5	0.950	C19—C20	1.368 (5)
C6—C7	1.357 (4)	C19—H19	0.950
C6—C11	1.486 (4)	C20—C21	1.376 (5)
C7—C8	1.398 (4)	C20—H20	0.950
C7—H7	0.950	C21—C22	1.372 (4)
C8—C9	1.409 (4)	C21—H21	0.950
C9—C10	1.354 (4)	C22—H22	0.950
C9—H9	0.950	C23—C24	1.378 (4)
C10—H10	0.950	C23—C28	1.382 (4)
C11—F1	1.339 (3)	C24—C25	1.378 (4)
C11—F2	1.358 (3)	C24—H24	0.950
C11—C12	1.528 (4)	C25—C26	1.368 (5)
C12—F4	1.336 (3)	C25—H25	0.950
C12—F3	1.337 (3)	C26—C27	1.369 (4)
C12—C13	1.546 (4)	C26—H26	0.950
C13—F6	1.332 (4)	C27—C28	1.378 (4)

C13—F5	1.337 (4)	C27—H27	0.950
C13—C14	1.537 (4)	C28—H28	0.950
C14—F7	1.320 (3)		

C17—P1—C23	104.75 (13)	F8—C14—C13	108.1 (2)
C17—P1—C1	100.35 (12)	F7—C14—C15	108.3 (3)
C23—P1—C1	103.01 (12)	F8—C14—C15	107.7 (2)
C2—C1—C10	119.4 (2)	C13—C14—C15	114.5 (3)
C2—C1—P1	118.22 (19)	F10—C15—F9	109.5 (3)
C10—C1—P1	122.4 (2)	F10—C15—C16	108.1 (3)
C1—C2—C3	120.6 (2)	F9—C15—C16	105.9 (3)
C1—C2—C2^{i}	118.9 (2)	F10—C15—C14	109.7 (3)
C3—C2—C2^{i}	120.4 (2)	F9—C15—C14	108.3 (3)
C4—C3—C2	123.1 (2)	C16—C15—C14	115.1 (3)
C4—C3—C8	117.7 (2)	F12—C16—F13	106.7 (3)
C2—C3—C8	119.2 (2)	F12—C16—F11	107.2 (3)
C5—C4—C3	121.8 (2)	F13—C16—F11	109.3 (3)
C5—C4—H4	119.1	F12—C16—C15	111.7 (3)
C3—C4—H4	119.1	F13—C16—C15	109.9 (3)
C4—C5—C6	120.0 (3)	F11—C16—C15	111.8 (3)
C4—C5—H5	120.0	C22—C17—C18	118.7 (3)
C6—C5—H5	120.0	C22—C17—P1	124.1 (2)
C7—C6—C5	119.9 (2)	C18—C17—P1	117.2 (2)
C7—C6—C11	120.4 (2)	C19—C18—C17	120.4 (3)
C5—C6—C11	119.7 (3)	C19—C18—H18	119.8
C6—C7—C8	121.0 (2)	C17—C18—H18	119.8
C6—C7—H7	119.5	C20—C19—C18	120.4 (3)
C8—C7—H7	119.5	C20—C19—H19	119.8
C7—C8—C9	121.7 (2)	C18—C19—H19	119.8
C7—C8—C3	119.7 (2)	C19—C20—C21	119.7 (3)
C9—C8—C3	118.7 (2)	C19—C20—H20	120.1
C10—C9—C8	120.9 (2)	C21—C20—H20	120.1
C10—C9—H9	119.6	C22—C21—C20	120.0 (3)
C8—C9—H9	119.6	C22—C21—H21	120.0
C9—C10—C1	121.1 (3)	C20—C21—H21	120.0
C9—C10—H10	119.4	C21—C22—C17	120.7 (3)
C1—C10—H10	119.4	C21—C22—H22	119.6
F1—C11—F2	106.6 (2)	C17—C22—H22	119.6
F1—C11—C6	111.3 (2)	C24—C23—C28	118.8 (3)
F2—C11—C6	110.7 (2)	C24—C23—P1	116.3 (2)
F1—C11—C12	106.9 (2)	C28—C23—P1	124.6 (2)
F2—C11—C12	106.5 (2)	C25—C24—C23	120.7 (3)
C6—C11—C12	114.3 (2)	C25—C24—H24	119.7
F4—C12—F3	108.0 (2)	C23—C24—H24	119.7
F4—C12—C11	107.8 (2)	C26—C25—C24	120.1 (3)
F3—C12—C11	108.1 (2)	C26—C25—H25	120.0
F4—C12—C13	105.0 (2)	C24—C25—H25	120.0
F3—C12—C13	107.4 (2)	C25—C26—C27	119.8 (3)

C11—C12—C13	120.0 (2)	C25—C26—H26	120.1
F6—C13—F5	107.6 (3)	C27—C26—H26	120.1
F6—C13—C14	108.5 (3)	C26—C27—C28	120.4 (3)
F5—C13—C14	107.6 (2)	C26—C27—H27	119.8
F6—C13—C12	108.4 (2)	C28—C27—H27	119.8
F5—C13—C12	106.1 (2)	C27—C28—C23	120.2 (3)
C14—C13—C12	118.2 (3)	C27—C28—H28	119.9
F7—C14—F8	108.2 (3)	C23—C28—H28	119.9
F7—C14—C13	109.8 (2)		

C17—P1—C1—C2	−83.5 (2)	C11—C12—C13—C14	−60.0 (4)
C23—P1—C1—C2	168.5 (2)	F6—C13—C14—F7	−164.4 (2)
C17—P1—C1—C10	97.9 (2)	F5—C13—C14—F7	79.4 (3)
C23—P1—C1—C10	−10.0 (3)	C12—C13—C14—F7	−40.6 (4)
C10—C1—C2—C3	−1.5 (4)	F6—C13—C14—F8	−46.5 (3)
P1—C1—C2—C3	179.88 (19)	F5—C13—C14—F8	−162.6 (2)
C10—C1—C2—C2^{i}	176.4 (2)	C12—C13—C14—F8	77.4 (3)
P1—C1—C2—C2^{i}	−2.2 (3)	F6—C13—C14—C15	73.5 (3)
C1—C2—C3—C4	−177.6 (3)	F5—C13—C14—C15	−42.6 (3)
C2^{i}—C2—C3—C4	4.5 (4)	C12—C13—C14—C15	−162.6 (3)
C1—C2—C3—C8	2.6 (4)	F7—C14—C15—F10	−168.4 (3)
C2^{i}—C2—C3—C8	−175.4 (2)	F8—C14—C15—F10	74.8 (3)
C2—C3—C4—C5	179.8 (3)	C13—C14—C15—F10	−45.5 (4)
C8—C3—C4—C5	−0.3 (4)	F7—C14—C15—F9	−48.8 (4)
C3—C4—C5—C6	0.7 (4)	F8—C14—C15—F9	−165.7 (3)
C4—C5—C6—C7	0.1 (4)	C13—C14—C15—F9	74.0 (4)
C4—C5—C6—C11	179.8 (3)	F7—C14—C15—C16	69.4 (4)
C5—C6—C7—C8	−1.1 (4)	F8—C14—C15—C16	−47.4 (4)
C11—C6—C7—C8	179.1 (2)	C13—C14—C15—C16	−167.7 (3)
C6—C7—C8—C9	−177.4 (3)	F10—C15—C16—F12	−55.7 (4)
C6—C7—C8—C3	1.4 (4)	F9—C15—C16—F12	−173.1 (3)
C4—C3—C8—C7	−0.7 (4)	C14—C15—C16—F12	67.4 (4)
C2—C3—C8—C7	179.2 (2)	F10—C15—C16—F13	62.5 (4)
C4—C3—C8—C9	178.2 (2)	F9—C15—C16—F13	−54.8 (4)
C2—C3—C8—C9	−1.9 (4)	C14—C15—C16—F13	−174.4 (3)
C7—C8—C9—C10	179.2 (3)	F10—C15—C16—F11	−175.8 (3)
C3—C8—C9—C10	0.3 (4)	F9—C15—C16—F11	66.8 (4)
C8—C9—C10—C1	0.8 (4)	C14—C15—C16—F11	−52.7 (4)
C2—C1—C10—C9	−0.2 (4)	C23—P1—C17—C22	66.8 (3)
P1—C1—C10—C9	178.4 (2)	C1—P1—C17—C22	−39.8 (3)
C7—C6—C11—F1	−148.6 (3)	C23—P1—C17—C18	−116.7 (2)
C5—C6—C11—F1	31.6 (4)	C1—P1—C17—C18	136.8 (2)
C7—C6—C11—F2	−30.2 (4)	C22—C17—C18—C19	−0.5 (4)
C5—C6—C11—F2	150.1 (3)	P1—C17—C18—C19	−177.2 (2)
C7—C6—C11—C12	90.1 (3)	C17—C18—C19—C20	−0.3 (5)
C5—C6—C11—C12	−89.7 (3)	C18—C19—C20—C21	0.7 (5)
F1—C11—C12—F4	−178.6 (2)	C19—C20—C21—C22	−0.4 (5)
F2—C11—C12—F4	67.6 (3)	C20—C21—C22—C17	−0.4 (5)

C6—C11—C12—F4	−54.9 (3)	C18—C17—C22—C21	0.8 (4)
F1—C11—C12—F3	−62.2 (3)	P1—C17—C22—C21	177.3 (2)
F2—C11—C12—F3	−175.9 (2)	C17—P1—C23—C24	176.5 (2)
C6—C11—C12—F3	61.5 (3)	C1—P1—C23—C24	−78.9 (2)
F1—C11—C12—C13	61.4 (3)	C17—P1—C23—C28	2.2 (3)
F2—C11—C12—C13	−52.4 (3)	C1—P1—C23—C28	106.8 (3)
C6—C11—C12—C13	−174.9 (2)	C28—C23—C24—C25	0.0 (4)
F4—C12—C13—F6	−57.6 (3)	P1—C23—C24—C25	−174.7 (2)
F3—C12—C13—F6	−172.3 (2)	C23—C24—C25—C26	−0.3 (4)
C11—C12—C13—F6	63.8 (4)	C24—C25—C26—C27	0.5 (5)
F4—C12—C13—F5	57.8 (3)	C25—C26—C27—C28	−0.5 (5)
F3—C12—C13—F5	−56.9 (3)	C26—C27—C28—C23	0.2 (5)
C11—C12—C13—F5	179.2 (3)	C24—C23—C28—C27	0.0 (4)
F4—C12—C13—C14	178.6 (2)	P1—C23—C28—C27	174.2 (2)
F3—C12—C13—C14	63.8 (3)		

Symmetry code: (i) $-x+1, y, -z+1/2$.