Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1,1′-Bis(diphenylphosphino)cobaltocenium tetrafluoridoborate

Jian-Guo Hou,[a]* Pu Zhang,[a] Chen Ye[b] and Tie-Gang Yu[b]

[a]Department of Biotic Environment, Nanchang Institute of Technology, Nanchang 330013, People's Republic of China, and [b]Key Laboratory of Pesticides & Chemical Biology, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China
Correspondence e-mail: hjg0715@yahoo.com.cn

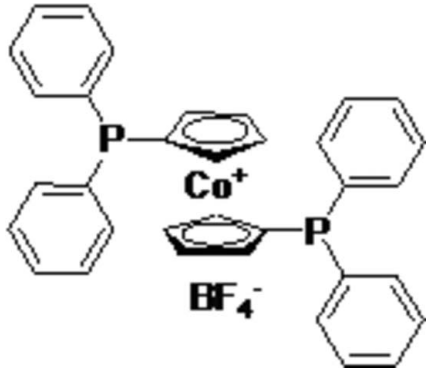
Received 4 September 2007; accepted 2 October 2007

Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.005 Å; disorder in solvent or counterion; R factor = 0.045; wR factor = 0.124; data-to-parameter ratio = 14.5.

The title compound, $[Co(C_{17}H_{14}P)_2]BF_4$, was obtained by the anion exchange of 1,1′-bis(diphenylphosphino)cobaltocenium chloride with sodium tetrafluoroborate. Both the cation and anion lie on crystallographic twofold axes which run through the Co^{III} ion, and both the B atom and one F atom of the anion, respectively. Three of the F atoms of the BF_4^- anion are disordered equally over two sites. The two diphenylphosphine ligands are *trans* to each other with respect to the Co^{III} ion. The crystal structure contains weak C—H···F interactions.

Related literature

The structure of a related compound containing the same cation with a nitrate anion has already been determined (Brasse *et al.*, 2000)



Experimental

Crystal data

$[Co(C_{17}H_{14}P)_2]BF_4$
M_r = 644.24
Monoclinic, $C2/c$
a = 10.3357 (11) Å
b = 13.1659 (14) Å
c = 22.894 (3) Å
β = 102.085 (2)°
V = 3046.3 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.72 mm^{-1}
T = 297 (2) K
0.20 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.870, T_{max} = 0.932
10252 measured reflections
2970 independent reflections
2655 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
S = 1.08
2970 reflections
205 parameters
21 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···F1^{i}	0.93	2.78	3.473 (8)	132

Symmetry code: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors acknowledge financial support from the National Natural Science Foundation of China (No. 20572029), New Century Excellent Talents in Universities (NCET-04-0743), and the Cultivation Fund of the Key Scientific and Technical Innovation Project, Ministry of Education of China (No. 705039).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2500).

References

Brasse, C. C., Englert, U. & Salzer, A. (2000). *Organometallics*, **19**, 3818–3823.
Bruker (2001). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2001). *SHELXTL*. Version 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2004). *SADABS*. University of Göttingen, Germany.

  doi:10.1107/S1600536807048404

supplementary materials

Acta Cryst. (2007). E**63**, m2730 [**doi:10.1107/S1600536807048404**]

1,1'-Bis(diphenylphosphino)cobaltocenium tetrafluoridoborate

J.-G. Hou, P. Zhang, C. Ye and T.-G. Yu

Comment

The molecular structure of the title complex consists of a [(η5-Ph2PC5H4)2Co]+ cation and a $BF4^{-}$ anion (Fig.1), in which the bond length and angles of the cation are similar to those in the cation of the complex 1,1'-Bis(diphenylphosphino)cobaltocenium nitrate (Brasse *et al.*, 2000). The two Ph_2P– substituents are *trans* to each other with respect to the Co^{III} metal center, and the two substituted cyclopentadienyl rings are exactly staggered with a dihedral angle of 4.62 (18)° between them. The distance between the atom Co1 and the center of the unique cyclopentadienyl ring is 1.6380 (13) Å. In the crystal structutre, molecules are linked by C—H···F hydrogen bonds, as shown in Fig.2.

Experimental

The title compound was obtained by anion exchange of 1,1'-Bis(diphenylphosphino)cobaltocenium chloride with 1.2 equiv of sodium tetrafluoroborate. Crystals appropriate for data collection were obtained by slow diffusion of hexane into a solution of the the title compound in dichloromethane at 293 K.

Refinement

F1, F3 and F4 are disordered equally over two sites imposed by the crystallographic twofold symmetry. All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H = 0.93 Å; with U_{iso}(H) = 1.2U_{eq}(C).

Figures

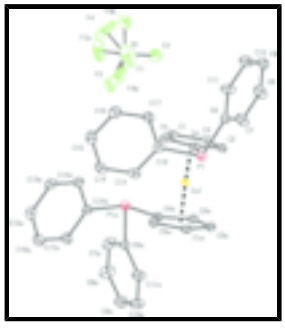


Fig. 1. The molecular structure with atom labels and 50% probability displacement ellipsoids for non-H atoms. H atoms are represented by circles of arbitrary size [Symmetry codes: (*a*) −*x* + 2, *y*, −*z* + 3/2; (*b*) −*x* + 1, *y*, −*z* + 3/2]

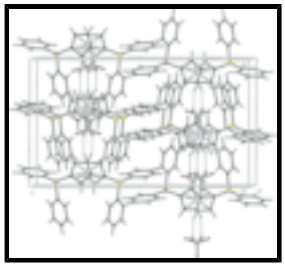


Fig. 2. A partial packing plot showing C—H···F hydrogen bonds as dashed lines.

1,1'-Bis(diphenylphosphino)cobaltocenium tetrafluoridoborate

Crystal data

$[Co(C_{17}H_{14}P)_2]BF_4$	F_{000} = 1320
M_r = 644.24	D_x = 1.405 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 5457 reflections
a = 10.3357 (11) Å	θ = 2.5–27.7º
b = 13.1659 (14) Å	μ = 0.72 mm^{-1}
c = 22.894 (3) Å	*T* = 297 (2) K
β = 102.085 (2)º	Block, yellow
V = 3046.3 (6) Å^3	0.20 × 0.15 × 0.10 mm
Z = 4	

Data collection

Bruker SMART CCD diffractometer	2970 independent reflections
Radiation source: fine-focus sealed tube	2655 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.025
T = 297(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	*h* = −12→12
T_{min} = 0.870, T_{max} = 0.932	*k* = −14→16
10252 measured reflections	*l* = −28→28

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.045	H-atom parameters constrained
$wR(F^2)$ = 0.125	$w = 1/[\sigma^2(F_o^2) + (0.0776P)^2 + 1.0622P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.08	$(\Delta/\sigma)_{max} < 0.001$
2970 reflections	$\Delta\rho_{max}$ = 0.49 e Å^{-3}

205 parameters
21 restraints
Primary atom site location: structure-invariant direct methods

$\Delta\rho_{min} = -0.36$ e Å^{-3}
Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Co1	1.0000	0.60723 (4)	0.7500	0.04454 (19)	
C1	0.8097 (3)	0.5865 (3)	0.75876 (13)	0.0610 (7)	
H1	0.7821	0.5677	0.7934	0.073*	
C2	0.8716 (3)	0.6816 (2)	0.68594 (12)	0.0560 (6)	
H2	0.8923	0.7370	0.6644	0.067*	
C3	0.8290 (3)	0.6865 (3)	0.74086 (12)	0.0625 (8)	
H3	0.8161	0.7453	0.7614	0.075*	
C4	0.8773 (2)	0.5777 (2)	0.66922 (11)	0.0512 (6)	
C5	0.8394 (3)	0.5192 (2)	0.71517 (12)	0.0547 (6)	
H5	0.8350	0.4487	0.7163	0.066*	
C6	0.7918 (3)	0.5732 (2)	0.54478 (12)	0.0550 (6)	
C7	0.8100 (4)	0.5751 (4)	0.48680 (15)	0.0909 (12)	
H7	0.8920	0.5583	0.4789	0.109*	
C8	0.7070 (5)	0.6020 (4)	0.44030 (16)	0.1003 (15)	
H8	0.7202	0.6005	0.4014	0.120*	
C9	0.5890 (4)	0.6299 (3)	0.45003 (16)	0.0822 (10)	
H9	0.5215	0.6495	0.4184	0.099*	
C10	0.5690 (4)	0.6292 (4)	0.50737 (16)	0.0979 (13)	
H10	0.4872	0.6479	0.5147	0.117*	
C11	0.6702 (3)	0.6007 (3)	0.55444 (14)	0.0847 (12)	
H11	0.6553	0.6003	0.5931	0.102*	
C12	0.9059 (3)	0.3975 (2)	0.60954 (12)	0.0565 (7)	
C13	1.0036 (3)	0.3419 (3)	0.64705 (15)	0.0732 (9)	
H13	1.0812	0.3741	0.6660	0.088*	
C14	0.9876 (4)	0.2396 (3)	0.65664 (17)	0.0830 (10)	
H14	1.0526	0.2042	0.6831	0.100*	
C15	0.8761 (4)	0.1899 (3)	0.62734 (17)	0.0826 (10)	
H15	0.8656	0.1209	0.6336	0.099*	
C16	0.7805 (4)	0.2427 (3)	0.58887 (19)	0.0899 (11)	

H16	0.7054	0.2091	0.5684	0.108*	
C17	0.7948 (3)	0.3462 (3)	0.58021 (16)	0.0761 (9)	
H17	0.7286	0.3813	0.5543	0.091*	
F2	0.5000	0.5484 (2)	0.7500	0.1305 (15)	
F1	0.5209 (12)	0.4095 (5)	0.6985 (2)	0.185 (6)	0.50
F3	0.6174 (8)	0.4195 (4)	0.7881 (2)	0.107 (2)	0.50
P1	0.93254 (7)	0.53398 (6)	0.60262 (3)	0.0569 (2)	
B1	0.5000	0.4466 (4)	0.7500	0.094 (2)	
F4	0.4042 (9)	0.4033 (5)	0.7672 (8)	0.317 (12)	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co1	0.0398 (3)	0.0519 (3)	0.0405 (3)	0.000	0.00524 (19)	0.000
C1	0.0407 (13)	0.090 (2)	0.0538 (15)	−0.0025 (13)	0.0125 (11)	−0.0118 (14)
C2	0.0492 (14)	0.0613 (16)	0.0508 (13)	0.0057 (12)	−0.0052 (11)	0.0007 (12)
C3	0.0472 (14)	0.076 (2)	0.0590 (15)	0.0143 (13)	−0.0010 (12)	−0.0162 (14)
C4	0.0425 (13)	0.0651 (16)	0.0431 (12)	−0.0036 (11)	0.0027 (10)	−0.0061 (11)
C5	0.0462 (14)	0.0655 (17)	0.0526 (14)	−0.0099 (12)	0.0112 (11)	−0.0079 (12)
C6	0.0581 (16)	0.0617 (16)	0.0456 (13)	−0.0003 (13)	0.0119 (11)	0.0014 (12)
C7	0.095 (3)	0.127 (3)	0.0565 (18)	0.042 (2)	0.0282 (18)	0.0230 (19)
C8	0.111 (3)	0.143 (4)	0.0494 (17)	0.035 (3)	0.0231 (19)	0.033 (2)
C9	0.081 (2)	0.100 (3)	0.0605 (18)	0.007 (2)	0.0026 (16)	0.0174 (18)
C10	0.061 (2)	0.164 (4)	0.064 (2)	0.016 (2)	0.0030 (16)	−0.006 (2)
C11	0.0602 (19)	0.147 (4)	0.0454 (15)	0.002 (2)	0.0074 (13)	−0.0117 (17)
C12	0.0556 (16)	0.0687 (17)	0.0460 (13)	0.0071 (13)	0.0122 (11)	−0.0065 (11)
C13	0.0581 (18)	0.082 (2)	0.0757 (19)	0.0142 (16)	0.0054 (15)	−0.0075 (17)
C14	0.076 (2)	0.086 (2)	0.086 (2)	0.025 (2)	0.0140 (18)	0.0068 (19)
C15	0.101 (3)	0.068 (2)	0.085 (2)	0.0096 (19)	0.033 (2)	0.0035 (18)
C16	0.086 (3)	0.081 (2)	0.096 (3)	−0.014 (2)	0.004 (2)	−0.004 (2)
C17	0.072 (2)	0.074 (2)	0.0731 (19)	0.0005 (17)	−0.0060 (16)	0.0015 (16)
F2	0.108 (3)	0.0566 (19)	0.212 (5)	0.000	−0.001 (3)	0.000
F1	0.324 (16)	0.137 (6)	0.061 (3)	0.028 (7)	−0.039 (5)	−0.030 (3)
F3	0.142 (5)	0.078 (3)	0.086 (3)	0.007 (3)	−0.008 (4)	0.030 (3)
P1	0.0520 (4)	0.0738 (5)	0.0455 (4)	−0.0011 (3)	0.0112 (3)	−0.0050 (3)
B1	0.084 (4)	0.048 (3)	0.147 (7)	0.000	0.020 (4)	0.000
F4	0.167 (9)	0.086 (5)	0.79 (4)	−0.038 (6)	0.302 (17)	−0.067 (14)

Geometric parameters (Å, °)

Co1—C2^{i}	2.014 (3)	C10—C11	1.387 (5)
Co1—C2	2.014 (2)	C10—H10	0.9300
Co1—C3^{i}	2.025 (3)	C11—H11	0.9300
Co1—C3	2.025 (3)	C12—C17	1.380 (4)
Co1—C1^{i}	2.037 (3)	C12—C13	1.390 (4)
Co1—C1	2.037 (3)	C12—P1	1.830 (3)
Co1—C5	2.044 (3)	C13—C14	1.380 (5)
Co1—C5^{i}	2.044 (3)	C13—H13	0.9300

Co1—C4	2.049 (2)	C14—C15	1.372 (5)
Co1—C4^{i}	2.049 (2)	C14—H14	0.9300
C1—C3	1.406 (5)	C15—C16	1.368 (5)
C1—C5	1.415 (4)	C15—H15	0.9300
C1—H1	0.9300	C16—C17	1.388 (6)
C2—C3	1.418 (4)	C16—H16	0.9300
C2—C4	1.424 (4)	C17—H17	0.9300
C2—H2	0.9300	F2—B1	1.341 (5)
C3—H3	0.9300	F1—F4^{ii}	0.985 (15)
C4—C5	1.424 (4)	F1—B1	1.336 (6)
C4—P1	1.829 (3)	F1—F3^{ii}	1.529 (11)
C5—H5	0.9300	F3—F4^{ii}	1.257 (17)
C6—C11	1.370 (5)	F3—B1	1.385 (5)
C6—C7	1.379 (4)	F3—F1^{ii}	1.529 (11)
C6—P1	1.825 (3)	B1—F4^{ii}	1.274 (5)
C7—C8	1.385 (5)	B1—F4	1.274 (5)
C7—H7	0.9300	B1—F1^{ii}	1.336 (6)
C8—C9	1.336 (6)	B1—F3^{ii}	1.385 (5)
C8—H8	0.9300	F4—F1^{ii}	0.985 (14)
C9—C10	1.371 (5)	F4—F3^{ii}	1.257 (17)
C9—H9	0.9300		
C2^{i}—Co1—C2	121.84 (16)	C4—C5—Co1	69.82 (15)
C2^{i}—Co1—C3^{i}	41.10 (11)	C1—C5—H5	125.8
C2—Co1—C3^{i}	104.64 (12)	C4—C5—H5	125.8
C2^{i}—Co1—C3	104.64 (12)	Co1—C5—H5	126.6
C2—Co1—C3	41.10 (11)	C11—C6—C7	117.7 (3)
C3^{i}—Co1—C3	118.0 (2)	C11—C6—P1	125.2 (2)
C2^{i}—Co1—C1^{i}	68.54 (13)	C7—C6—P1	117.1 (2)
C2—Co1—C1^{i}	119.76 (12)	C6—C7—C8	120.5 (4)
C3^{i}—Co1—C1^{i}	40.49 (13)	C6—C7—H7	119.8
C3—Co1—C1^{i}	154.01 (14)	C8—C7—H7	119.8
C2^{i}—Co1—C1	119.76 (12)	C9—C8—C7	121.6 (3)
C2—Co1—C1	68.54 (13)	C9—C8—H8	119.2
C3^{i}—Co1—C1	154.01 (14)	C7—C8—H8	119.2
C3—Co1—C1	40.49 (13)	C8—C9—C10	118.9 (3)
C1^{i}—Co1—C1	164.57 (19)	C8—C9—H9	120.6
C2^{i}—Co1—C5	156.51 (11)	C10—C9—H9	120.6
C2—Co1—C5	68.53 (12)	C9—C10—C11	120.4 (4)
C3^{i}—Co1—C5	162.18 (11)	C9—C10—H10	119.8
C3—Co1—C5	68.41 (13)	C11—C10—H10	119.8
C1^{i}—Co1—C5	127.39 (13)	C6—C11—C10	120.9 (3)
C1—Co1—C5	40.58 (11)	C6—C11—H11	119.5
C2^{i}—Co1—C5^{i}	68.53 (12)	C10—C11—H11	119.5

C2—Co1—C5^{i}	156.51 (11)	C17—C12—C13	117.7 (3)
C3^{i}—Co1—C5^{i}	68.41 (13)	C17—C12—P1	124.3 (2)
C3—Co1—C5^{i}	162.18 (11)	C13—C12—P1	117.9 (2)
C1^{i}—Co1—C5^{i}	40.58 (11)	C14—C13—C12	121.1 (3)
C1—Co1—C5^{i}	127.39 (13)	C14—C13—H13	119.4
C5—Co1—C5^{i}	110.94 (17)	C12—C13—H13	119.4
C2^{i}—Co1—C4	159.80 (12)	C15—C14—C13	120.3 (3)
C2—Co1—C4	41.04 (11)	C15—C14—H14	119.9
C3^{i}—Co1—C4	123.55 (11)	C13—C14—H14	119.9
C3—Co1—C4	69.06 (11)	C16—C15—C14	119.4 (4)
C1^{i}—Co1—C4	108.27 (12)	C16—C15—H15	120.3
C1—Co1—C4	68.63 (11)	C14—C15—H15	120.3
C5—Co1—C4	40.71 (11)	C15—C16—C17	120.4 (4)
C5^{i}—Co1—C4	122.90 (12)	C15—C16—H16	119.8
C2^{i}—Co1—C4^{i}	41.04 (11)	C17—C16—H16	119.8
C2—Co1—C4^{i}	159.80 (12)	C12—C17—C16	120.9 (3)
C3^{i}—Co1—C4^{i}	69.06 (11)	C12—C17—H17	119.5
C3—Co1—C4^{i}	123.55 (11)	C16—C17—H17	119.5
C1^{i}—Co1—C4^{i}	68.63 (11)	F4^{ii}—F1—B1	64.6 (6)
C1—Co1—C4^{i}	108.27 (12)	F4^{ii}—F1—F3^{ii}	117.3 (11)
C5—Co1—C4^{i}	122.90 (12)	B1—F1—F3^{ii}	57.3 (4)
C5^{i}—Co1—C4^{i}	40.71 (11)	F4^{ii}—F3—B1	57.4 (4)
C4—Co1—C4^{i}	158.15 (17)	F4^{ii}—F3—F1^{ii}	102.2 (7)
C3—C1—C5	108.4 (3)	B1—F3—F1^{ii}	54.3 (3)
C3—C1—Co1	69.32 (16)	C6—P1—C4	100.10 (13)
C5—C1—Co1	69.99 (15)	C6—P1—C12	103.26 (13)
C3—C1—H1	125.8	C4—P1—C12	99.10 (13)
C5—C1—H1	125.8	F4^{ii}—B1—F4	126.8 (7)
Co1—C1—H1	126.5	F4—B1—F1	112.9 (5)
C3—C2—C4	108.7 (3)	F4^{ii}—B1—F1^{ii}	112.9 (5)
C3—C2—Co1	69.89 (15)	F1—B1—F1^{ii}	137.2 (8)
C4—C2—Co1	70.79 (15)	F4^{ii}—B1—F2	116.6 (4)
C3—C2—H2	125.7	F4—B1—F2	116.6 (4)
C4—C2—H2	125.7	F1—B1—F2	111.4 (4)
Co1—C2—H2	125.2	F1^{ii}—B1—F2	111.4 (4)
C1—C3—C2	107.8 (3)	F4^{ii}—B1—F3^{ii}	109.0 (6)
C1—C3—Co1	70.20 (16)	F4—B1—F3^{ii}	56.2 (7)
C2—C3—Co1	69.01 (15)	F1—B1—F3^{ii}	68.4 (4)
C1—C3—H3	126.1	F1^{ii}—B1—F3^{ii}	100.4 (4)
C2—C3—H3	126.1	F2—B1—F3^{ii}	104.9 (3)
Co1—C3—H3	126.2	F4^{ii}—B1—F3	56.2 (7)
C5—C4—C2	106.7 (2)	F4—B1—F3	109.0 (6)
C5—C4—P1	128.9 (2)	F1—B1—F3	100.4 (4)

C2—C4—P1	124.4 (2)	F1^{ii}—B1—F3	68.4 (4)
C5—C4—Co1	69.48 (14)	F2—B1—F3	104.9 (3)
C2—C4—Co1	68.17 (13)	F3^{ii}—B1—F3	150.2 (6)
P1—C4—Co1	124.76 (14)	F1^{ii}—F4—F3^{ii}	137.2 (8)
C1—C5—C4	108.5 (3)	F1^{ii}—F4—B1	71.1 (5)
C1—C5—Co1	69.43 (16)	F3^{ii}—F4—B1	66.3 (5)
C2^{i}—Co1—C1—C3	77.22 (19)	C3—C1—C5—C4	−0.2 (3)
C2—Co1—C1—C3	−38.13 (16)	Co1—C1—C5—C4	−59.09 (18)
C3^{i}—Co1—C1—C3	41.1 (4)	C3—C1—C5—Co1	58.86 (19)
C1^{i}—Co1—C1—C3	−163.60 (16)	C2—C4—C5—C1	0.6 (3)
C5—Co1—C1—C3	−119.8 (2)	P1—C4—C5—C1	177.5 (2)
C5^{i}—Co1—C1—C3	161.84 (16)	Co1—C4—C5—C1	58.85 (18)
C4—Co1—C1—C3	−82.37 (18)	C2—C4—C5—Co1	−58.21 (17)
C4^{i}—Co1—C1—C3	120.65 (17)	P1—C4—C5—Co1	118.7 (2)
C2^{i}—Co1—C1—C5	−163.02 (17)	C2^{i}—Co1—C5—C1	39.5 (4)
C2—Co1—C1—C5	81.62 (19)	C2—Co1—C5—C1	−81.7 (2)
C3^{i}—Co1—C1—C5	160.9 (2)	C3^{i}—Co1—C5—C1	−152.0 (4)
C3—Co1—C1—C5	119.8 (2)	C3—Co1—C5—C1	−37.31 (19)
C1^{i}—Co1—C1—C5	−43.85 (17)	C1^{i}—Co1—C5—C1	166.59 (18)
C5^{i}—Co1—C1—C5	−78.4 (3)	C5^{i}—Co1—C5—C1	123.6 (2)
C4—Co1—C1—C5	37.39 (18)	C4—Co1—C5—C1	−119.9 (3)
C4^{i}—Co1—C1—C5	−119.60 (18)	C4^{i}—Co1—C5—C1	79.6 (2)
C2^{i}—Co1—C2—C3	−74.98 (17)	C2^{i}—Co1—C5—C4	159.4 (3)
C3^{i}—Co1—C2—C3	−116.0 (2)	C2—Co1—C5—C4	38.22 (17)
C1^{i}—Co1—C2—C3	−156.9 (2)	C3^{i}—Co1—C5—C4	−32.1 (5)
C1—Co1—C2—C3	37.58 (18)	C3—Co1—C5—C4	82.57 (19)
C5—Co1—C2—C3	81.33 (19)	C1^{i}—Co1—C5—C4	−73.5 (2)
C5^{i}—Co1—C2—C3	174.7 (3)	C1—Co1—C5—C4	119.9 (3)
C4—Co1—C2—C3	119.3 (2)	C5^{i}—Co1—C5—C4	−116.56 (18)
C4^{i}—Co1—C2—C3	−47.1 (4)	C4^{i}—Co1—C5—C4	−160.57 (16)
C2^{i}—Co1—C2—C4	165.76 (18)	C11—C6—C7—C8	−1.4 (6)
C3^{i}—Co1—C2—C4	124.74 (18)	P1—C6—C7—C8	178.6 (4)
C3—Co1—C2—C4	−119.3 (2)	C6—C7—C8—C9	2.2 (8)
C1^{i}—Co1—C2—C4	83.86 (19)	C7—C8—C9—C10	−1.7 (7)
C1—Co1—C2—C4	−81.68 (18)	C8—C9—C10—C11	0.5 (7)
C5—Co1—C2—C4	−37.93 (16)	C7—C6—C11—C10	0.2 (6)
C5^{i}—Co1—C2—C4	55.4 (4)	P1—C6—C11—C10	−179.8 (3)
C4^{i}—Co1—C2—C4	−166.3 (2)	C9—C10—C11—C6	0.3 (7)
C5—C1—C3—C2	−0.3 (3)	C17—C12—C13—C14	−2.8 (5)
Co1—C1—C3—C2	58.99 (18)	P1—C12—C13—C14	176.9 (3)
C5—C1—C3—Co1	−59.27 (19)	C12—C13—C14—C15	2.5 (5)
C4—C2—C3—C1	0.7 (3)	C13—C14—C15—C16	−0.5 (6)
Co1—C2—C3—C1	−59.73 (19)	C14—C15—C16—C17	−1.1 (6)

C4—C2—C3—Co1	60.42 (17)	C13—C12—C17—C16	1.2 (5)
C2^{i}—Co1—C3—C1	−118.95 (17)	P1—C12—C17—C16	−178.5 (3)
C2—Co1—C3—C1	119.1 (2)	C15—C16—C17—C12	0.7 (6)
C3^{i}—Co1—C3—C1	−160.95 (18)	C11—C6—P1—C4	−15.3 (3)
C1^{i}—Co1—C3—C1	170.13 (17)	C7—C6—P1—C4	164.7 (3)
C5—Co1—C3—C1	37.40 (16)	C11—C6—P1—C12	86.7 (3)
C5^{i}—Co1—C3—C1	−54.0 (5)	C7—C6—P1—C12	−93.3 (3)
C4—Co1—C3—C1	81.23 (18)	C5—C4—P1—C6	111.3 (2)
C4^{i}—Co1—C3—C1	−78.61 (19)	C2—C4—P1—C6	−72.3 (2)
C2^{i}—Co1—C3—C2	122.0 (2)	Co1—C4—P1—C6	−158.04 (18)
C3^{i}—Co1—C3—C2	80.00 (17)	C5—C4—P1—C12	6.0 (3)
C1^{i}—Co1—C3—C2	51.1 (3)	C2—C4—P1—C12	−177.6 (2)
C1—Co1—C3—C2	−119.1 (2)	Co1—C4—P1—C12	96.62 (19)
C5—Co1—C3—C2	−81.65 (18)	C17—C12—P1—C6	−5.8 (3)
C5^{i}—Co1—C3—C2	−173.1 (4)	C13—C12—P1—C6	174.5 (2)
C4—Co1—C3—C2	−37.83 (17)	C17—C12—P1—C4	96.9 (3)
C4^{i}—Co1—C3—C2	162.34 (17)	C13—C12—P1—C4	−82.8 (3)
C3—C2—C4—C5	−0.8 (3)	F3^{ii}—F1—B1—F4^{ii}	155.2 (9)
Co1—C2—C4—C5	59.04 (18)	F4^{ii}—F1—B1—F4	−119.9 (9)
C3—C2—C4—P1	−177.90 (19)	F3^{ii}—F1—B1—F4	35.3 (7)
Co1—C2—C4—P1	−118.04 (19)	F4^{ii}—F1—B1—F1^{ii}	−73.4 (7)
C3—C2—C4—Co1	−59.85 (17)	F3^{ii}—F1—B1—F1^{ii}	81.8 (4)
C2^{i}—Co1—C4—C5	−156.0 (3)	F4^{ii}—F1—B1—F2	106.6 (7)
C2—Co1—C4—C5	−118.7 (2)	F3^{ii}—F1—B1—F2	−98.2 (4)
C3^{i}—Co1—C4—C5	168.73 (18)	F4^{ii}—F1—B1—F3^{ii}	−155.2 (9)
C3—Co1—C4—C5	−80.83 (19)	F4^{ii}—F1—B1—F3	−4.0 (8)
C1^{i}—Co1—C4—C5	126.65 (18)	F3^{ii}—F1—B1—F3	151.2 (6)
C1—Co1—C4—C5	−37.28 (18)	F1^{ii}—F3—B1—F4^{ii}	−140.2 (6)
C5^{i}—Co1—C4—C5	84.3 (2)	F4^{ii}—F3—B1—F4	122.2 (9)
C4^{i}—Co1—C4—C5	48.63 (15)	F1^{ii}—F3—B1—F4	−18.0 (8)
C2^{i}—Co1—C4—C2	−37.3 (5)	F4^{ii}—F3—B1—F1	3.4 (7)
C3^{i}—Co1—C4—C2	−72.6 (2)	F1^{ii}—F3—B1—F1	−136.8 (8)
C3—Co1—C4—C2	37.89 (18)	F4^{ii}—F3—B1—F1^{ii}	140.2 (6)
C1^{i}—Co1—C4—C2	−114.64 (18)	F4^{ii}—F3—B1—F2	−112.3 (4)
C1—Co1—C4—C2	81.44 (19)	F1^{ii}—F3—B1—F2	107.5 (4)
C5—Co1—C4—C2	118.7 (2)	F4^{ii}—F3—B1—F3^{ii}	67.7 (4)
C5^{i}—Co1—C4—C2	−156.99 (17)	F1^{ii}—F3—B1—F3^{ii}	−72.5 (4)
C4^{i}—Co1—C4—C2	167.35 (16)	F4^{ii}—B1—F4—F1^{ii}	85.9 (7)
C2^{i}—Co1—C4—P1	80.3 (4)	F1—B1—F4—F1^{ii}	135.0 (10)
C2—Co1—C4—P1	117.5 (3)	F2—B1—F4—F1^{ii}	−94.1 (7)
C3^{i}—Co1—C4—P1	45.0 (2)	F3^{ii}—B1—F4—F1^{ii}	175.2 (10)
C3—Co1—C4—P1	155.4 (2)	F3—B1—F4—F1^{ii}	24.4 (9)

C1^{i}—Co1—C4—P1	2.9 (2)	F4^{ii}—B1—F4—F3^{ii}	−89.4 (5)
C1—Co1—C4—P1	−161.0 (2)	F1—B1—F4—F3^{ii}	−40.2 (6)
C5—Co1—C4—P1	−123.8 (3)	F1^{ii}—B1—F4—F3^{ii}	−175.2 (10)
C5^{i}—Co1—C4—P1	−39.5 (2)	F2—B1—F4—F3^{ii}	90.6 (5)
C4^{i}—Co1—C4—P1	−75.14 (17)	F3—B1—F4—F3^{ii}	−150.9 (6)

Symmetry codes: (i) −*x*+2, *y*, −*z*+3/2; (ii) −*x*+1, *y*, −*z*+3/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···F1^{iii}	0.93	2.78	3.473 (8)	132

Symmetry codes: (iii) −*x*+3/2, *y*+1/2, −*z*+3/2.

Fig. 1

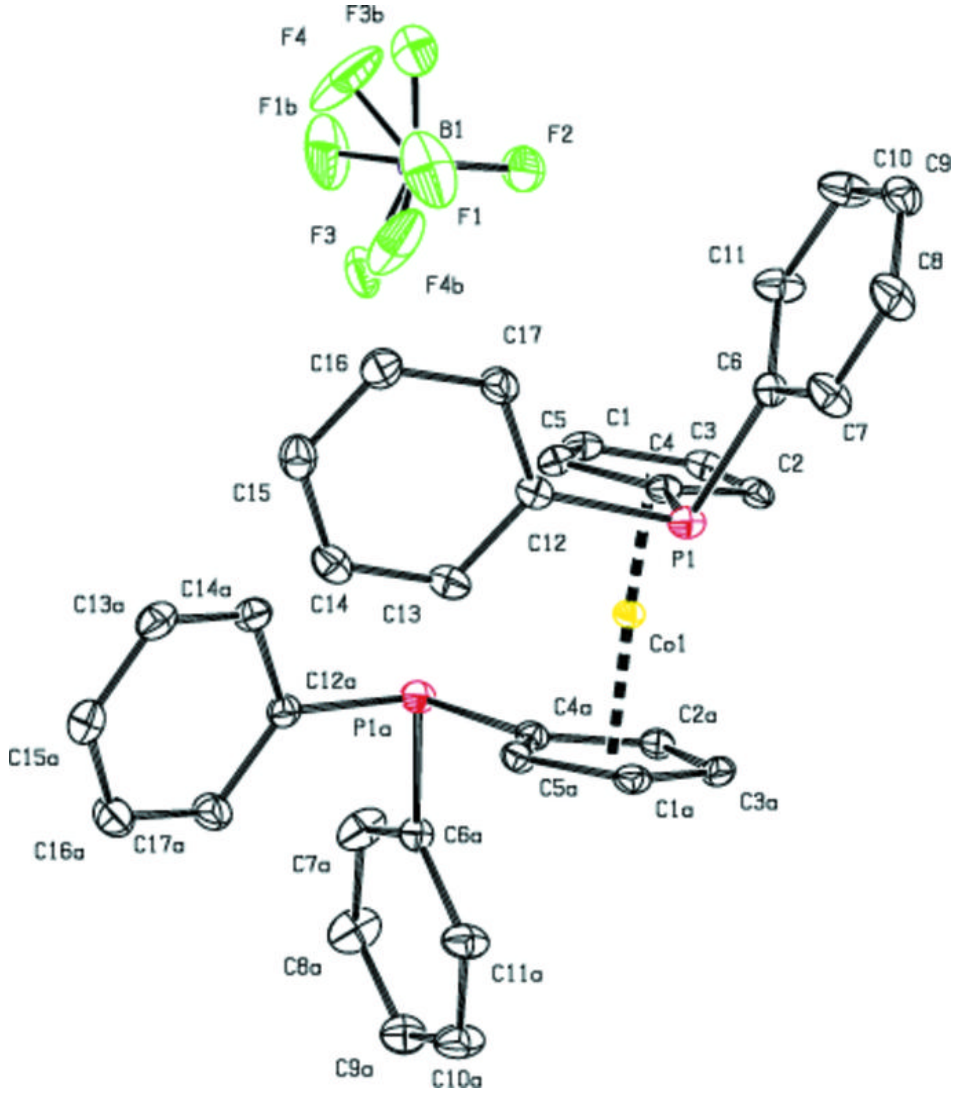

F3b
F4
F1b
B1
F2
F3
F1
F4b
C10
C9
C11
C8
C17
C16
C6
C5
C1
C4
C3
C7
C2
C15
C12
P1
C14a
C13a
C14
C13
Co1
C12a
C4a
C2a
P1a
C15a
C5a
C1a
C3a
C16a
C17a
C6a
C7a
C8a
C11a
C9a
C10a

Fig. 2