

Dichlorido[2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl- κ C¹]bis(trimethylphosphine- κ P)cobalt(III)

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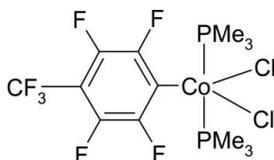
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.013$ Å; disorder in main residue; R factor = 0.061; wR factor = 0.186; data-to-parameter ratio = 15.1.

In the title compound, $[\text{Co}(\text{C}_7\text{F}_7)\text{Cl}_2(\text{C}_3\text{H}_9\text{P})_2]$, the Co^{III} atom displays a trigonal-bipyramidal coordination geometry, with the two Cl ligands and the C atom of the perfluorotolyl ligand in the equatorial plane and the two phosphine ligands occupying axial positions. The molecule has an approximate C_{2v} symmetry. The trifluoromethyl group is disordered over two positions, with nearly equal occupancies.

Related literature

For general background on the activation of C–F bonds and the formation of C–C bonds, see: Schaub *et al.* (2006); Böhm *et al.* (2001); Zheng *et al.* (2009).



Experimental

Crystal data

$[\text{Co}(\text{C}_7\text{F}_7)\text{Cl}_2(\text{C}_3\text{H}_9\text{P})_2]$
 $M_r = 499.04$
 Orthorhombic, $Pbca$
 $a = 12.3321$ (19) Å

$b = 13.3657$ (19) Å
 $c = 25.426$ (4) Å
 $V = 4190.8$ (11) Å³
 $Z = 8$

Mo $K\alpha$ radiation
 $\mu = 1.28$ mm⁻¹

$T = 293$ K
 $0.25 \times 0.20 \times 0.18$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
 $T_{\text{min}} = 0.740$, $T_{\text{max}} = 0.802$

18353 measured reflections
 3373 independent reflections
 2345 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.052$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.186$
 $S = 1.07$
 3373 reflections
 223 parameters

8 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.78$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.69$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Cl1–Co1	1.987 (6)	Co1–P1	2.262 (2)
Cl1–Co1	2.2290 (18)	Co1–P2	2.264 (2)
Cl2–Co1	2.2613 (16)		
Cl1–Co1–Cl1	123.2 (2)	Cl2–Co1–P1	90.03 (7)
Cl1–Co1–Cl2	125.5 (2)	Cl1–Co1–P2	89.93 (19)
Cl1–Co1–Cl2	111.29 (7)	Cl1–Co1–P2	89.13 (8)
Cl1–Co1–P1	89.36 (19)	Cl2–Co1–P2	90.86 (7)
Cl1–Co1–P1	90.78 (8)	P1–Co1–P2	179.08 (8)

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GK2264).

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supplementary materials

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Dichlorido[2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl- κC^1]bis(trimethylphosphine- κP)cobalt(III)

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Comment

The activation of C—F bonds by transition metal compounds has blossomed in the past few years. There has also been considerable interest in the chemistry of carbon-fluorine bond cleavage followed by carbon-carbon bond formation because they play a key role in the organic synthesis (Schaub *et al.*, 2006; Böhm *et al.*, 2001). Recently we have reported the stoichiometric reaction involving one-electron oxidative addition of bromobenzene and (1-perflurotoluene- κC)tris(trimethylphosphine- κP)cobalt gaining bromo(1-perflurotoluene- κC)tris(trimethylphosphine- κP)cobalt and C—C coupling product (Zheng *et al.*, 2009). We tried to synthesise the compound 1, through the reaction of bromopentafluorobenzene with the(1-perflurotoluene- κC)tris(trimethylphosphine- κP)cobalt. We added the solution of hydrochloric acid in order to abolish the organometallic compounds and gain the organic compound 1. Surprisingly we isolated complex 2 (Scheme 2) as red crystals and its molecular structure is shown in Fig.1. The cobalt atom displays a trigonal bipyramidal coordination, with two Cl atoms and C atom in the equatorial plane and two P atoms occupying axial positions. The Cl1—Co1 and Cl2—Co1 distances are 2.2290 (18) Å and 2.2613 (16) Å, respectively. The angle between the phosphine ligands and the Co atom, P1—Co1—P2 is 179.08 (8)°.

Experimental

The reaction leading to the title compound is shown in Scheme 2. To a solution of 1 (0.50 g, 1.00 mmol) in 30 mL of pentane was added bromopentafluorobenzene (0.74 g, 3.00 mmol) with stirring at 213 K. The mixture was allowed to warm-up to 293 K and was stirred for 18 h. The color changed from green to yellow-brown. The reaction mixture was added to a solution of hydrochloric acid with a color change to red-brown. Pentane was used to extract the organic product. Crystallization from pentane at 273 K afforded the title compound as red crystals in 37% yield.

Refinement

Hydrogen atoms were included in the refinement at calculated positions (C—H = 0.97 Å) and treated as riding, with $U_{iso}(H) = 1.5 U_{eq}(C)$. In the refinement process, the sum of the occupancy factors of the disordered CF₃ groups was constrained to 1.0 and restraints were imposed on its geometry [C—C 1.54 (2) Å; C—F 1.36 (2) Å]. The occupancy factor of the major orientation of the CF₃ group refined at 0.513 (13).

Figures

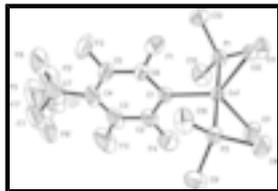


Fig. 1. Molecular structure and atom numbering scheme for the title compound with the displacement ellipsoids shown at the 30% probability level.

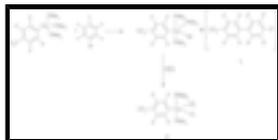


Fig. 2. Preparation of the title compound.

Dichlorido[2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl- κC^1]bis(trimethylphosphine- κP)cobalt(III)

Crystal data

[Co(C₇F₇)Cl₂(C₃H₉P)₂]

$M_r = 499.04$

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

$a = 12.3321$ (19) Å

$b = 13.3657$ (19) Å

$c = 25.426$ (4) Å

$V = 4190.8$ (11) Å³

$Z = 8$

$F(000) = 2000$

$D_x = 1.582$ Mg m⁻³

Melting point: 380 K

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2967 reflections

$\theta = 2.3$ – 21.0°

$\mu = 1.28$ mm⁻¹

$T = 293$ K

Block, red

$0.25 \times 0.20 \times 0.18$ mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.740$, $T_{\max} = 0.802$

18353 measured reflections

3373 independent reflections

2345 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.052$

$\theta_{\max} = 24.2^\circ$, $\theta_{\min} = 2.3^\circ$

$h = -14 \rightarrow 10$

$k = -15 \rightarrow 12$

$l = -27 \rightarrow 29$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.061$

$wR(F^2) = 0.186$

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

$S = 1.07$	$w = 1/[\sigma^2(F_o^2) + (0.0935P)^2 + 7.5678P]$
3373 reflections	where $P = (F_o^2 + 2F_c^2)/3$
223 parameters	$(\Delta/\sigma)_{\max} = 0.013$
8 restraints	$\Delta\rho_{\max} = 0.78 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\min} = -0.69 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.9572 (5)	0.1013 (5)	0.1322 (3)	0.0593 (16)	
C2	0.9141 (7)	0.1728 (6)	0.0990 (3)	0.080 (2)	
C3	0.8099 (8)	0.1731 (9)	0.0813 (3)	0.102 (3)	
C4	0.7378 (6)	0.0992 (11)	0.0944 (4)	0.109 (4)	
C5	0.7789 (7)	0.0239 (8)	0.1266 (3)	0.094 (3)	
C6	0.8834 (6)	0.0266 (6)	0.1449 (3)	0.073 (2)	
C8	1.3056 (6)	-0.0189 (6)	0.0919 (3)	0.087 (2)	
H8A	1.3203	-0.0538	0.1241	0.130*	
H8B	1.3477	0.0414	0.0907	0.130*	
H8C	1.3244	-0.0607	0.0626	0.130*	
C9	1.1447 (8)	0.0770 (7)	0.0268 (3)	0.101 (3)	
H9A	1.1794	0.1413	0.0286	0.151*	
H9B	1.0687	0.0858	0.0201	0.151*	
H9C	1.1766	0.0384	-0.0010	0.151*	
C10	1.0943 (7)	-0.1069 (5)	0.0800 (3)	0.087 (2)	
H10A	1.1015	-0.1461	0.1115	0.130*	
H10B	1.1264	-0.1422	0.0510	0.130*	
H10C	1.0189	-0.0954	0.0729	0.130*	
C11	1.1647 (6)	0.2311 (6)	0.2713 (3)	0.092 (3)	
H11A	1.2031	0.1723	0.2824	0.137*	
H11B	1.1369	0.2656	0.3016	0.137*	
H11C	1.2131	0.2744	0.2524	0.137*	
C12	0.9874 (8)	0.3117 (6)	0.2110 (4)	0.105 (3)	
H12A	1.0344	0.3495	0.1884	0.157*	
H12B	0.9727	0.3495	0.2423	0.157*	
H12C	0.9206	0.2979	0.1931	0.157*	
C13	0.9579 (7)	0.1302 (8)	0.2711 (3)	0.101 (3)	

supplementary materials

H13A	0.9885	0.0672	0.2816	0.151*	
H13B	0.8913	0.1187	0.2525	0.151*	
H13C	0.9438	0.1701	0.3017	0.151*	
C11	1.22875 (15)	0.22034 (13)	0.13739 (8)	0.0772 (6)	
C12	1.18147 (13)	-0.01081 (11)	0.21464 (6)	0.0566 (4)	
Co1	1.10845 (6)	0.10295 (6)	0.15914 (3)	0.0498 (3)	
F1	0.9169 (4)	-0.0490 (4)	0.17618 (19)	0.0965 (15)	
F2	0.7167 (4)	-0.0546 (6)	0.1418 (2)	0.146 (3)	
F3	0.7792 (5)	0.2497 (5)	0.0496 (2)	0.156 (3)	
F4	0.9791 (5)	0.2502 (4)	0.0832 (2)	0.1083 (16)	
P1	1.05246 (15)	0.19513 (14)	0.22862 (7)	0.0664 (5)	
P2	1.16269 (14)	0.01209 (14)	0.08875 (7)	0.0622 (5)	
C7	0.6149 (13)	0.0863 (14)	0.0797 (8)	0.106 (9)*	0.487 (13)
F6	0.5612 (14)	0.0191 (12)	0.1062 (6)	0.154 (7)*	0.487 (13)
F5	0.5737 (12)	0.1839 (12)	0.0899 (6)	0.138 (6)*	0.487 (13)
F7	0.6077 (13)	0.0920 (13)	0.0284 (6)	0.150 (6)*	0.487 (13)
C7'	0.6232 (14)	0.1080 (15)	0.0695 (8)	0.141 (12)*	0.513 (13)
F6'	0.6148 (12)	0.1727 (13)	0.0306 (6)	0.158 (6)*	0.513 (13)
F7'	0.6005 (11)	0.0140 (10)	0.0511 (5)	0.133 (5)*	0.513 (13)
F5'	0.5527 (11)	0.1180 (11)	0.1069 (5)	0.131 (5)*	0.513 (13)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.046 (4)	0.069 (4)	0.062 (4)	0.006 (3)	-0.001 (3)	-0.001 (3)
C2	0.072 (5)	0.092 (6)	0.077 (5)	0.023 (5)	-0.004 (4)	0.012 (4)
C3	0.078 (6)	0.152 (9)	0.074 (5)	0.056 (7)	-0.024 (5)	-0.011 (6)
C4	0.042 (4)	0.209 (12)	0.076 (6)	0.027 (6)	-0.010 (4)	-0.035 (7)
C5	0.052 (5)	0.157 (9)	0.072 (5)	-0.024 (6)	0.013 (4)	-0.030 (6)
C6	0.053 (4)	0.095 (6)	0.072 (5)	-0.008 (4)	0.003 (4)	0.004 (4)
C8	0.055 (4)	0.104 (6)	0.101 (6)	0.014 (4)	0.009 (4)	-0.010 (5)
C9	0.121 (7)	0.113 (7)	0.068 (5)	0.018 (6)	0.002 (5)	0.006 (5)
C10	0.083 (6)	0.072 (5)	0.105 (6)	0.012 (4)	-0.018 (5)	-0.019 (4)
C11	0.075 (5)	0.096 (6)	0.103 (6)	0.012 (5)	-0.017 (5)	-0.031 (5)
C12	0.111 (7)	0.081 (6)	0.122 (7)	0.042 (5)	-0.003 (6)	-0.018 (5)
C13	0.078 (6)	0.148 (8)	0.078 (5)	-0.005 (6)	0.021 (4)	-0.005 (5)
C11	0.0681 (11)	0.0602 (10)	0.1034 (14)	-0.0203 (9)	0.0083 (10)	0.0143 (9)
C12	0.0546 (9)	0.0522 (9)	0.0629 (9)	0.0059 (7)	-0.0052 (7)	0.0159 (7)
Co1	0.0414 (5)	0.0477 (5)	0.0603 (5)	0.0008 (3)	0.0002 (4)	0.0075 (4)
F1	0.088 (3)	0.098 (3)	0.103 (3)	-0.031 (3)	-0.006 (3)	0.027 (3)
F2	0.076 (3)	0.227 (7)	0.136 (5)	-0.073 (5)	0.010 (3)	-0.025 (5)
F3	0.138 (5)	0.199 (6)	0.130 (5)	0.083 (5)	-0.048 (4)	0.023 (4)
F4	0.112 (4)	0.089 (3)	0.124 (4)	0.017 (3)	-0.012 (3)	0.042 (3)
P1	0.0549 (11)	0.0721 (12)	0.0723 (11)	0.0116 (9)	0.0003 (9)	-0.0081 (9)
P2	0.0544 (10)	0.0683 (11)	0.0638 (11)	0.0091 (9)	-0.0010 (8)	0.0011 (8)

Geometric parameters (\AA , $^\circ$)

C1—C2	1.382 (10)	C10—H10C	0.9600
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C1—C6	1.389 (10)	C11—P1	1.823 (8)
C1—Co1	1.987 (6)	C11—H11A	0.9600
C2—C3	1.362 (12)	C11—H11B	0.9600
C2—F4	1.369 (9)	C11—H11C	0.9600
C3—F3	1.358 (11)	C12—P1	1.808 (8)
C3—C4	1.370 (15)	C12—H12A	0.9600
C4—C5	1.393 (14)	C12—H12B	0.9600
C4—C7'	1.554 (17)	C12—H12C	0.9600
C4—C7	1.570 (16)	C13—P1	1.811 (8)
C5—F2	1.357 (11)	C13—H13A	0.9600
C5—C6	1.370 (11)	C13—H13B	0.9600
C6—F1	1.350 (9)	C13—H13C	0.9600
C8—P2	1.812 (7)	Cl1—Co1	2.2290 (18)
C8—H8A	0.9600	Cl2—Co1	2.2613 (16)
C8—H8B	0.9600	Co1—P1	2.262 (2)
C8—H8C	0.9600	Co1—P2	2.264 (2)
C9—P2	1.812 (8)	C7—F6	1.302 (16)
C9—H9A	0.9600	C7—F7	1.311 (17)
C9—H9B	0.9600	C7—F5	1.424 (17)
C9—H9C	0.9600	C7'—F5'	1.296 (17)
C10—P2	1.814 (8)	C7'—F6'	1.317 (17)
C10—H10A	0.9600	C7'—F7'	1.368 (17)
C10—H10B	0.9600		
C2—C1—C6	112.8 (7)	P1—C12—H12B	109.5
C2—C1—Co1	124.3 (6)	H12A—C12—H12B	109.5
C6—C1—Co1	122.9 (5)	P1—C12—H12C	109.5
C3—C2—F4	117.0 (8)	H12A—C12—H12C	109.5
C3—C2—C1	124.5 (9)	H12B—C12—H12C	109.5
F4—C2—C1	118.5 (7)	P1—C13—H13A	109.5
F3—C3—C2	117.5 (11)	P1—C13—H13B	109.5
F3—C3—C4	120.4 (9)	H13A—C13—H13B	109.5
C2—C3—C4	122.1 (9)	P1—C13—H13C	109.5
C3—C4—C5	115.3 (7)	H13A—C13—H13C	109.5
C3—C4—C7'	115.9 (12)	H13B—C13—H13C	109.5
C5—C4—C7'	128.7 (13)	C1—Co1—Cl1	123.2 (2)
C3—C4—C7	130.4 (12)	C1—Co1—Cl2	125.5 (2)
C5—C4—C7	114.3 (12)	Cl1—Co1—Cl2	111.29 (7)
C7'—C4—C7	14.8 (11)	C1—Co1—P1	89.36 (19)
F2—C5—C6	117.1 (9)	Cl1—Co1—P1	90.78 (8)
F2—C5—C4	121.3 (8)	Cl2—Co1—P1	90.03 (7)
C6—C5—C4	121.6 (9)	C1—Co1—P2	89.93 (19)
F1—C6—C5	118.0 (8)	Cl1—Co1—P2	89.13 (8)
F1—C6—C1	118.3 (6)	Cl2—Co1—P2	90.86 (7)
C5—C6—C1	123.8 (8)	P1—Co1—P2	179.08 (8)
P2—C8—H8A	109.5	C12—P1—C13	105.9 (5)
P2—C8—H8B	109.5	C12—P1—C11	104.9 (4)
H8A—C8—H8B	109.5	C13—P1—C11	105.1 (4)
P2—C8—H8C	109.5	C12—P1—Co1	114.3 (3)
H8A—C8—H8C	109.5	C13—P1—Co1	113.6 (3)

supplementary materials

H8B—C8—H8C	109.5	C11—P1—Co1	112.1 (3)
P2—C9—H9A	109.5	C9—P2—C8	105.5 (4)
P2—C9—H9B	109.5	C9—P2—C10	104.9 (4)
H9A—C9—H9B	109.5	C8—P2—C10	104.9 (4)
P2—C9—H9C	109.5	C9—P2—Co1	113.2 (3)
H9A—C9—H9C	109.5	C8—P2—Co1	112.0 (3)
H9B—C9—H9C	109.5	C10—P2—Co1	115.5 (3)
P2—C10—H10A	109.5	F6—C7—F7	121.3 (17)
P2—C10—H10B	109.5	F6—C7—F5	110.9 (16)
H10A—C10—H10B	109.5	F7—C7—F5	96.0 (15)
P2—C10—H10C	109.5	F6—C7—C4	116.3 (16)
H10A—C10—H10C	109.5	F7—C7—C4	107.2 (14)
H10B—C10—H10C	109.5	F5—C7—C4	101.6 (13)
P1—C11—H11A	109.5	F5'—C7'—F6'	115.5 (17)
P1—C11—H11B	109.5	F5'—C7'—F7'	102.1 (16)
H11A—C11—H11B	109.5	F6'—C7'—F7'	109.3 (16)
P1—C11—H11C	109.5	F5'—C7'—C4	108.5 (15)
H11A—C11—H11C	109.5	F6'—C7'—C4	115.3 (16)
H11B—C11—H11C	109.5	F7'—C7'—C4	104.8 (14)
P1—C12—H12A	109.5		
C6—C1—C2—C3	1.7 (11)	C1—Co1—P1—C12	-57.7 (4)
Co1—C1—C2—C3	-178.6 (6)	C11—Co1—P1—C12	65.5 (4)
C6—C1—C2—F4	-179.5 (7)	C12—Co1—P1—C12	176.8 (4)
Co1—C1—C2—F4	0.2 (10)	C1—Co1—P1—C13	64.1 (4)
F4—C2—C3—F3	0.1 (12)	C11—Co1—P1—C13	-172.7 (3)
C1—C2—C3—F3	178.9 (7)	C12—Co1—P1—C13	-61.4 (3)
F4—C2—C3—C4	179.7 (8)	C1—Co1—P1—C11	-176.9 (4)
C1—C2—C3—C4	-1.5 (14)	C11—Co1—P1—C11	-53.7 (3)
F3—C3—C4—C5	179.1 (7)	C12—Co1—P1—C11	57.6 (3)
C2—C3—C4—C5	-0.4 (13)	C1—Co1—P2—C9	63.6 (4)
F3—C3—C4—C7'	1.8 (15)	C11—Co1—P2—C9	-59.6 (4)
C2—C3—C4—C7'	-177.8 (11)	C12—Co1—P2—C9	-170.8 (4)
F3—C3—C4—C7	-2.0 (17)	C1—Co1—P2—C8	-177.3 (4)
C2—C3—C4—C7	178.5 (12)	C11—Co1—P2—C8	59.6 (3)
C3—C4—C5—F2	-178.9 (8)	C12—Co1—P2—C8	-51.7 (3)
C7'—C4—C5—F2	-1.9 (16)	C1—Co1—P2—C10	-57.3 (3)
C7—C4—C5—F2	2.0 (14)	C11—Co1—P2—C10	179.5 (3)
C3—C4—C5—C6	2.0 (13)	C12—Co1—P2—C10	68.2 (3)
C7'—C4—C5—C6	179.0 (12)	C3—C4—C7—F6	-166.9 (13)
C7—C4—C5—C6	-177.1 (10)	C5—C4—C7—F6	12.0 (19)
F2—C5—C6—F1	0.5 (11)	C7'—C4—C7—F6	180 (5)
C4—C5—C6—F1	179.6 (7)	C3—C4—C7—F7	54 (2)
F2—C5—C6—C1	179.0 (7)	C5—C4—C7—F7	-127.5 (14)
C4—C5—C6—C1	-1.8 (13)	C7'—C4—C7—F7	40 (4)
C2—C1—C6—F1	178.4 (7)	C3—C4—C7—F5	-46.5 (19)
Co1—C1—C6—F1	-1.3 (10)	C5—C4—C7—F5	132.4 (12)
C2—C1—C6—C5	-0.1 (11)	C7'—C4—C7—F5	-60 (4)
Co1—C1—C6—C5	-179.8 (6)	C3—C4—C7'—F5'	-118.0 (15)
C2—C1—Co1—C11	-1.3 (7)	C5—C4—C7'—F5'	65 (2)

supplementary materials

C6—C1—Co1—C11	178.4 (5)	C7—C4—C7'—F5'	51 (4)
C2—C1—Co1—C12	178.8 (5)	C3—C4—C7'—F6'	13 (2)
C6—C1—Co1—C12	-1.5 (7)	C5—C4—C7'—F6'	-163.6 (13)
C2—C1—Co1—P1	89.2 (6)	C7—C4—C7'—F6'	-178 (5)
C6—C1—Co1—P1	-91.1 (6)	C3—C4—C7'—F7'	133.6 (13)
C2—C1—Co1—P2	-90.2 (6)	C5—C4—C7'—F7'	-43.3 (19)
C6—C1—Co1—P2	89.5 (6)	C7—C4—C7'—F7'	-58 (4)

Fig. 2

