

trans-Tetracarbonylbis[tris(4-fluorophenyl)phosphane- κP]chromium(0)

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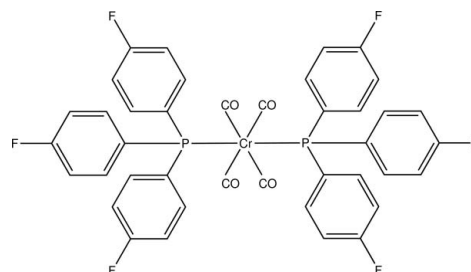
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.026; wR factor = 0.074; data-to-parameter ratio = 20.8.

In the title compound, $[\text{Cr}(\text{C}_{18}\text{H}_{12}\text{F}_3\text{P})_2(\text{CO})_4]$, the Cr atom is octahedrally coordinated by four carbonyl ligands and the two tertiary phosphanes that are *trans* to each other. The Cr atom and two carbonyl groups are on a twofold axis. The benzene rings attached to the phosphorus atom make dihedral angles of 80.32 (5), 52.91 (5) and 83.80 (5)° with each other. In the crystal, C—H \cdots O and C—H \cdots F intermolecular interactions form an infinite three-dimensional network.

Related literature

For the crystal structures of phosphane complexes of carbonylchromium compounds, see: Preston *et al.* (1972); bin Shawkataly *et al.* (1996, 2009). For related structures, see: Brunet *et al.* (2002); Bennett *et al.* (2004). A search of the Cambridge Structural Database (Allen, 2002) reveals 113 complexes of carbonylchromium complexes with bis-phosphanes. For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$[\text{Cr}(\text{C}_{18}\text{H}_{12}\text{F}_3\text{P})_2(\text{CO})_4]$
 $M_r = 796.53$
 Monoclinic, $C2/c$
 $a = 11.9318$ (8) Å
 $b = 18.0956$ (8) Å
 $c = 15.8195$ (8) Å
 $\beta = 92.740$ (1)°

$V = 3411.7$ (3) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.51$ mm⁻¹
 $T = 100$ K
 $0.29 \times 0.21 \times 0.19$ mm

Data collection

Bruker APEX Duo CCD
 area-detector diffractometer
 Absorption correction: multi-scan
 (SADABS; Bruker, 2009)
 $T_{\min} = 0.869$, $T_{\max} = 0.912$

35263 measured reflections
 5028 independent reflections
 4627 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.074$
 $S = 1.04$
 5028 reflections

242 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.42$ e Å⁻³
 $\Delta\rho_{\min} = -0.47$ e Å⁻³

Table 1

Selected bond lengths (Å).

Cr1—C37	1.8808 (17)	Cr1—C39	1.8989 (15)
Cr1—C38	1.8925 (11)	Cr1—P1	2.3331 (3)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4A \cdots O1 ⁱⁱ	0.93	2.55	3.4602 (16)	165
C8—H8A \cdots F1 ⁱⁱⁱ	0.93	2.48	3.3830 (16)	165
C14—H14A \cdots F3 ^{iv}	0.93	2.46	3.3561 (14)	161

Symmetry codes: (ii) $x + \frac{1}{2}, y - \frac{1}{2}, z$; (iii) $x - \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$; (iv) $-x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$.

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXTL (Sheldrick, 2008); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5213).

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supplementary materials

Acta Cryst. (2011). E67, m1314-m1315 [doi:10.1107/S1600536811033939]

***trans*-Tetracarbonylbis[tris(4-fluorophenyl)phosphane- κ P]chromium(0)**

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Comment

The bonding characteristics of metal carbonyls with a phosphane ligand in phosphane-substituted metal carbonyls are interesting. Several crystal structures of phosphane substituted group 6 carbonyls with *trans* coordination of phosphane are reported (Brunet *et al.* 2002; Bennett *et al.*, 2004).

In the title compound, the Cr—P bond lengths, with an average value of 2.3331 (3) Å (Table 1) are relatively short in spite of the presence of the bulky phosphane ligand compared to the average values of 2.3656 (16)Å in the complex *trans*-Cr(CO)₄(PPh₃)₂ (Bennett *et al.* 2004).

The Cr1, O1, O3, C37 C39 atoms lie on a twofold axis. The three benzene rings attached to the phosphorus atom make dihedral angles of 80.32 (5)° (between C1—C6 & C7—C12), 52.91 (5)° (between C1—C6 & C13—C18) and 83.80 (5)° (between C7—C12 & C13—C18) with each other.

In the crystal, the molecules are interconnected by intermolecular C4—H4A⋯O1ⁱⁱ, C8—H8A⋯F1ⁱⁱⁱ and C14—H14A⋯F3^{iv} interactions (Table 2) to form an infinite three-dimensional network (Fig. 2).

Experimental

All manipulations were performed under a dry, oxygen-free nitrogen atmosphere using standard Schlenk techniques. All solvents were dried over sodium under dry oxygen free nitrogen. Chromium hexacarbonyl (200 mg, 0.909 mmol) and tris(4-fluorophenyl)phosphane (301.8 mg, 0.9542 mmol) in 30 ml of pet ether (100–130°C) was refluxed for 12 h. Suitable single crystals were obtained by solvent-solvent diffusion in a mixture of dichloromethane/methanol.

Refinement

All hydrogen atoms were positioned geometrically and refined using a riding model with C—H = 0.93Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Figures

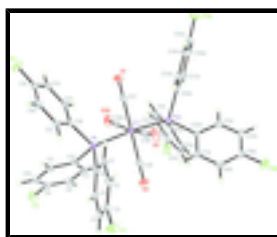


Fig. 1. The molecular structure, showing 50% probability displacement ellipsoids. Hydrogen atoms are shown as spheres of arbitrary radius.

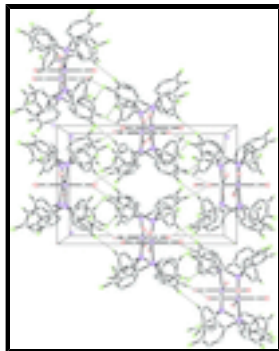


Fig. 2. The crystal packing of (I). Dashed lines indicate hydrogen bonds. H atoms not involved in the hydrogen bond interactions have been omitted for clarity.

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Crystal data

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$M_r = 796.53$

Monoclinic, $C2/c$

Hall symbol: $-C\ 2yc$

$a = 11.9318\ (8)\ \text{\AA}$

$b = 18.0956\ (8)\ \text{\AA}$

$c = 15.8195\ (8)\ \text{\AA}$

$\beta = 92.740\ (1)^\circ$

$V = 3411.7\ (3)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1616$

$D_x = 1.551\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 9233 reflections

$\theta = 2.4\text{--}30.1^\circ$

$\mu = 0.51\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Block, colourless

$0.29 \times 0.21 \times 0.19\ \text{mm}$

Data collection

Bruker APEX Duo CCD area-detector diffractometer

Radiation source: fine-focus sealed tube graphite

φ and ω scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2009)

$T_{\min} = 0.869$, $T_{\max} = 0.912$

35263 measured reflections

5028 independent reflections

4627 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.022$

$\theta_{\max} = 30.1^\circ$, $\theta_{\min} = 2.1^\circ$

$h = -16 \rightarrow 16$

$k = -25 \rightarrow 25$

$l = -22 \rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.026$

$wR(F^2) = 0.074$

$S = 1.04$

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

$w = 1/[\sigma^2(F_o^2) + (0.035P)^2 + 3.7272P]$

where $P = (F_o^2 + 2F_c^2)/3$

5028 reflections	$(\Delta/\sigma)_{\max} = 0.001$
242 parameters	$\Delta\rho_{\max} = 0.42 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\min} = -0.47 \text{ e } \text{\AA}^{-3}$

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Cr1	0.0000	0.470721 (12)	0.2500	0.01127 (6)
P1	0.18184 (2)	0.464307 (14)	0.310682 (16)	0.01170 (6)
F1	0.47047 (7)	0.30568 (5)	0.07445 (5)	0.03078 (18)
F2	0.27164 (8)	0.30623 (5)	0.63765 (5)	0.0368 (2)
F3	0.37981 (7)	0.75534 (4)	0.41277 (5)	0.02655 (16)
O1	0.0000	0.63797 (7)	0.2500	0.0450 (4)
O2	0.08864 (8)	0.48305 (6)	0.07365 (6)	0.0300 (2)
O3	0.0000	0.30234 (6)	0.2500	0.0249 (2)
C1	0.31342 (9)	0.45249 (6)	0.16868 (7)	0.01626 (19)
H1A	0.2919	0.5010	0.1573	0.020*
C2	0.37850 (9)	0.41494 (7)	0.11182 (7)	0.0195 (2)
H2A	0.4017	0.4379	0.0630	0.023*
C3	0.40757 (9)	0.34262 (7)	0.13002 (7)	0.0207 (2)
C4	0.37508 (10)	0.30617 (6)	0.20114 (7)	0.0207 (2)
H4A	0.3955	0.2572	0.2111	0.025*
C5	0.31090 (9)	0.34444 (6)	0.25788 (7)	0.01666 (19)
H5A	0.2883	0.3208	0.3064	0.020*
C6	0.27996 (8)	0.41807 (6)	0.24279 (6)	0.01374 (18)
C7	0.12666 (10)	0.36724 (6)	0.44384 (7)	0.0193 (2)
H7A	0.0583	0.3604	0.4142	0.023*
C8	0.14776 (11)	0.33051 (7)	0.52065 (8)	0.0247 (2)
H8A	0.0940	0.2998	0.5428	0.030*
C9	0.25007 (12)	0.34096 (6)	0.56260 (7)	0.0242 (2)
C10	0.33278 (10)	0.38535 (7)	0.53176 (7)	0.0231 (2)
H10A	0.4018	0.3906	0.5611	0.028*
C11	0.31014 (9)	0.42195 (6)	0.45570 (7)	0.0191 (2)
H11A	0.3647	0.4523	0.4340	0.023*

supplementary materials

C12	0.20668 (9)	0.41398 (6)	0.41100 (6)	0.01477 (18)
C13	0.19260 (9)	0.59837 (6)	0.39426 (7)	0.01655 (19)
H13A	0.1238	0.5831	0.4133	0.020*
C14	0.23616 (9)	0.66625 (6)	0.42015 (7)	0.0186 (2)
H14A	0.1979	0.6963	0.4567	0.022*
C15	0.33815 (10)	0.68791 (6)	0.39001 (7)	0.0185 (2)
C16	0.39903 (9)	0.64423 (6)	0.33799 (7)	0.0189 (2)
H16A	0.4679	0.6600	0.3195	0.023*
C17	0.35499 (9)	0.57552 (6)	0.31349 (7)	0.01725 (19)
H17A	0.3957	0.5448	0.2792	0.021*
C18	0.25037 (8)	0.55231 (5)	0.33991 (6)	0.01340 (17)
C37	0.0000	0.57466 (9)	0.2500	0.0235 (3)
C38	0.05647 (9)	0.47660 (6)	0.14043 (7)	0.0185 (2)
C39	0.0000	0.36578 (8)	0.2500	0.0154 (3)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.01065 (10)	0.00928 (10)	0.01385 (11)	0.000	0.00032 (7)	0.000
P1	0.01137 (11)	0.01041 (11)	0.01334 (12)	0.00025 (8)	0.00078 (8)	0.00089 (8)
F1	0.0299 (4)	0.0317 (4)	0.0315 (4)	0.0092 (3)	0.0101 (3)	-0.0112 (3)
F2	0.0589 (6)	0.0308 (4)	0.0198 (4)	-0.0033 (4)	-0.0080 (3)	0.0124 (3)
F3	0.0354 (4)	0.0177 (3)	0.0266 (4)	-0.0114 (3)	0.0022 (3)	-0.0056 (3)
O1	0.0433 (8)	0.0133 (6)	0.0749 (12)	0.000	-0.0335 (8)	0.000
O2	0.0223 (4)	0.0483 (6)	0.0196 (4)	-0.0018 (4)	0.0024 (3)	0.0089 (4)
O3	0.0365 (7)	0.0132 (5)	0.0250 (6)	0.000	0.0024 (5)	0.000
C1	0.0154 (4)	0.0155 (4)	0.0180 (5)	0.0012 (4)	0.0019 (4)	0.0001 (4)
C2	0.0173 (5)	0.0231 (5)	0.0185 (5)	0.0001 (4)	0.0042 (4)	-0.0012 (4)
C3	0.0165 (5)	0.0238 (5)	0.0221 (5)	0.0047 (4)	0.0020 (4)	-0.0085 (4)
C4	0.0213 (5)	0.0159 (5)	0.0245 (5)	0.0055 (4)	-0.0024 (4)	-0.0040 (4)
C5	0.0180 (5)	0.0142 (4)	0.0177 (4)	0.0018 (4)	-0.0011 (4)	-0.0002 (4)
C6	0.0121 (4)	0.0134 (4)	0.0156 (4)	0.0010 (3)	-0.0002 (3)	-0.0009 (3)
C7	0.0234 (5)	0.0168 (5)	0.0176 (5)	-0.0029 (4)	0.0008 (4)	0.0021 (4)
C8	0.0360 (6)	0.0184 (5)	0.0199 (5)	-0.0051 (5)	0.0023 (5)	0.0050 (4)
C9	0.0404 (7)	0.0168 (5)	0.0152 (5)	0.0029 (5)	-0.0016 (4)	0.0041 (4)
C10	0.0265 (5)	0.0227 (5)	0.0196 (5)	0.0039 (4)	-0.0050 (4)	0.0024 (4)
C11	0.0185 (5)	0.0204 (5)	0.0183 (5)	0.0009 (4)	-0.0007 (4)	0.0028 (4)
C12	0.0172 (4)	0.0126 (4)	0.0145 (4)	0.0017 (3)	0.0011 (3)	0.0010 (3)
C13	0.0157 (4)	0.0167 (5)	0.0174 (4)	-0.0012 (4)	0.0017 (3)	-0.0009 (4)
C14	0.0212 (5)	0.0167 (5)	0.0180 (5)	-0.0004 (4)	0.0012 (4)	-0.0038 (4)
C15	0.0244 (5)	0.0140 (4)	0.0168 (5)	-0.0054 (4)	-0.0022 (4)	-0.0004 (4)
C16	0.0184 (5)	0.0199 (5)	0.0185 (5)	-0.0062 (4)	0.0012 (4)	0.0004 (4)
C17	0.0157 (5)	0.0168 (5)	0.0194 (5)	-0.0020 (4)	0.0028 (4)	-0.0015 (4)
C18	0.0135 (4)	0.0121 (4)	0.0145 (4)	-0.0006 (3)	-0.0005 (3)	0.0008 (3)
C37	0.0188 (7)	0.0153 (7)	0.0350 (9)	0.000	-0.0117 (6)	0.000
C38	0.0138 (4)	0.0214 (5)	0.0200 (5)	-0.0004 (4)	-0.0013 (4)	0.0044 (4)
C39	0.0167 (6)	0.0159 (6)	0.0138 (6)	0.000	0.0013 (5)	0.000

Geometric parameters (Å, °)

Cr1—C37	1.8808 (17)	C5—C6	1.4001 (14)
Cr1—C38 ⁱ	1.8924 (11)	C5—H5A	0.9300
Cr1—C38	1.8925 (11)	C7—C12	1.3944 (15)
Cr1—C39	1.8989 (15)	C7—C8	1.3972 (15)
Cr1—P1 ⁱ	2.3331 (3)	C7—H7A	0.9300
Cr1—P1	2.3331 (3)	C8—C9	1.3744 (19)
P1—C6	1.8288 (10)	C8—H8A	0.9300
P1—C18	1.8391 (10)	C9—C10	1.3796 (18)
P1—C12	1.8414 (10)	C10—C11	1.3886 (15)
F1—C3	1.3587 (12)	C10—H10A	0.9300
F2—C9	1.3570 (13)	C11—C12	1.4005 (15)
F3—C15	1.3595 (12)	C11—H11A	0.9300
O1—C37	1.146 (2)	C13—C14	1.3880 (15)
O2—C38	1.1471 (15)	C13—C18	1.4020 (14)
O3—C39	1.1481 (19)	C13—H13A	0.9300
C1—C2	1.3931 (15)	C14—C15	1.3846 (16)
C1—C6	1.4023 (14)	C14—H14A	0.9300
C1—H1A	0.9300	C15—C16	1.3737 (16)
C2—C3	1.3806 (16)	C16—C17	1.3973 (15)
C2—H2A	0.9300	C16—H16A	0.9300
C3—C4	1.3758 (17)	C17—C18	1.3998 (14)
C4—C5	1.3918 (15)	C17—H17A	0.9300
C4—H4A	0.9300		
C37—Cr1—C38 ⁱ	86.78 (3)	C12—C7—C8	120.96 (11)
C37—Cr1—C38	86.78 (3)	C12—C7—H7A	119.5
C38 ⁱ —Cr1—C38	173.56 (7)	C8—C7—H7A	119.5
C37—Cr1—C39	180.0	C9—C8—C7	118.26 (11)
C38 ⁱ —Cr1—C39	93.22 (3)	C9—C8—H8A	120.9
C38—Cr1—C39	93.22 (3)	C7—C8—H8A	120.9
C37—Cr1—P1 ⁱ	92.850 (8)	F2—C9—C8	119.05 (11)
C38 ⁱ —Cr1—P1 ⁱ	90.85 (3)	F2—C9—C10	118.04 (11)
C38—Cr1—P1 ⁱ	89.47 (3)	C8—C9—C10	122.90 (11)
C39—Cr1—P1 ⁱ	87.150 (8)	C9—C10—C11	118.12 (11)
C37—Cr1—P1	92.851 (8)	C9—C10—H10A	120.9
C38 ⁱ —Cr1—P1	89.47 (3)	C11—C10—H10A	120.9
C38—Cr1—P1	90.85 (3)	C10—C11—C12	121.24 (11)
C39—Cr1—P1	87.149 (8)	C10—C11—H11A	119.4
P1 ⁱ —Cr1—P1	174.299 (16)	C12—C11—H11A	119.4
C6—P1—C18	104.74 (5)	C7—C12—C11	118.50 (10)
C6—P1—C12	101.46 (5)	C7—C12—P1	122.43 (8)
C18—P1—C12	99.22 (5)	C11—C12—P1	119.07 (8)
C6—P1—Cr1	112.95 (3)	C14—C13—C18	121.25 (10)
C18—P1—Cr1	117.00 (3)	C14—C13—H13A	119.4
C12—P1—Cr1	119.17 (3)	C18—C13—H13A	119.4

supplementary materials

C2—C1—C6	120.85 (10)	C15—C14—C13	118.16 (10)
C2—C1—H1A	119.6	C15—C14—H14A	120.9
C6—C1—H1A	119.6	C13—C14—H14A	120.9
C3—C2—C1	118.03 (10)	F3—C15—C16	118.55 (10)
C3—C2—H2A	121.0	F3—C15—C14	118.63 (10)
C1—C2—H2A	121.0	C16—C15—C14	122.81 (10)
F1—C3—C4	118.64 (10)	C15—C16—C17	118.40 (10)
F1—C3—C2	118.19 (11)	C15—C16—H16A	120.8
C4—C3—C2	123.17 (10)	C17—C16—H16A	120.8
C3—C4—C5	118.30 (10)	C16—C17—C18	120.86 (10)
C3—C4—H4A	120.9	C16—C17—H17A	119.6
C5—C4—H4A	120.9	C18—C17—H17A	119.6
C4—C5—C6	120.81 (10)	C17—C18—C13	118.45 (9)
C4—C5—H5A	119.6	C17—C18—P1	125.23 (8)
C6—C5—H5A	119.6	C13—C18—P1	116.31 (8)
C5—C6—C1	118.82 (9)	O1—C37—Cr1	180.0
C5—C6—P1	120.41 (8)	O2—C38—Cr1	177.10 (11)
C1—C6—P1	120.24 (8)	O3—C39—Cr1	180.0
C37—Cr1—P1—C6	-118.45 (4)	C7—C8—C9—C10	-0.71 (19)
C38 ⁱ —Cr1—P1—C6	154.80 (5)	F2—C9—C10—C11	-178.90 (11)
C38—Cr1—P1—C6	-31.63 (5)	C8—C9—C10—C11	1.24 (19)
C39—Cr1—P1—C6	61.55 (4)	C9—C10—C11—C12	-0.34 (18)
C37—Cr1—P1—C18	3.27 (4)	C8—C7—C12—C11	1.58 (17)
C38 ⁱ —Cr1—P1—C18	-83.48 (5)	C8—C7—C12—P1	-179.28 (9)
C38—Cr1—P1—C18	90.09 (5)	C10—C11—C12—C7	-1.03 (17)
C39—Cr1—P1—C18	-176.73 (4)	C10—C11—C12—P1	179.80 (9)
C37—Cr1—P1—C12	122.64 (4)	C6—P1—C12—C7	-111.54 (9)
C38 ⁱ —Cr1—P1—C12	35.89 (5)	C18—P1—C12—C7	141.25 (9)
C38—Cr1—P1—C12	-150.55 (5)	Cr1—P1—C12—C7	13.13 (10)
C39—Cr1—P1—C12	-57.36 (4)	C6—P1—C12—C11	67.60 (9)
C6—C1—C2—C3	0.94 (16)	C18—P1—C12—C11	-39.61 (9)
C1—C2—C3—F1	179.61 (10)	Cr1—P1—C12—C11	-167.73 (7)
C1—C2—C3—C4	0.20 (17)	C18—C13—C14—C15	0.74 (16)
F1—C3—C4—C5	179.83 (10)	C13—C14—C15—F3	177.88 (10)
C2—C3—C4—C5	-0.76 (18)	C13—C14—C15—C16	-2.03 (17)
C3—C4—C5—C6	0.18 (16)	F3—C15—C16—C17	-178.85 (10)
C4—C5—C6—C1	0.92 (16)	C14—C15—C16—C17	1.06 (17)
C4—C5—C6—P1	172.56 (8)	C15—C16—C17—C18	1.22 (16)
C2—C1—C6—C5	-1.49 (16)	C16—C17—C18—C13	-2.42 (16)
C2—C1—C6—P1	-173.15 (8)	C16—C17—C18—P1	178.79 (8)
C18—P1—C6—C5	130.53 (8)	C14—C13—C18—C17	1.42 (16)
C12—P1—C6—C5	27.68 (9)	C14—C13—C18—P1	-179.68 (8)
Cr1—P1—C6—C5	-101.07 (8)	C6—P1—C18—C17	0.15 (10)
C18—P1—C6—C1	-57.95 (9)	C12—P1—C18—C17	104.68 (9)
C12—P1—C6—C1	-160.80 (8)	Cr1—P1—C18—C17	-125.76 (8)
Cr1—P1—C6—C1	70.45 (9)	C6—P1—C18—C13	-178.66 (8)
C12—C7—C8—C9	-0.74 (18)	C12—P1—C18—C13	-74.13 (9)
C7—C8—C9—F2	179.43 (11)	Cr1—P1—C18—C13	55.42 (9)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
C4—H4A \cdots O1 ⁱⁱ	0.93	2.55	3.4602 (16)	165.
C8—H8A \cdots F1 ⁱⁱⁱ	0.93	2.48	3.3830 (16)	165.
C14—H14A \cdots F3 ^{iv}	0.93	2.46	3.3561 (14)	161.

Symmetry codes: (ii) $x+1/2, y-1/2, z$; (iii) $x-1/2, -y+1/2, z+1/2$; (iv) $-x+1/2, -y+3/2, -z+1$.

Fig. 1

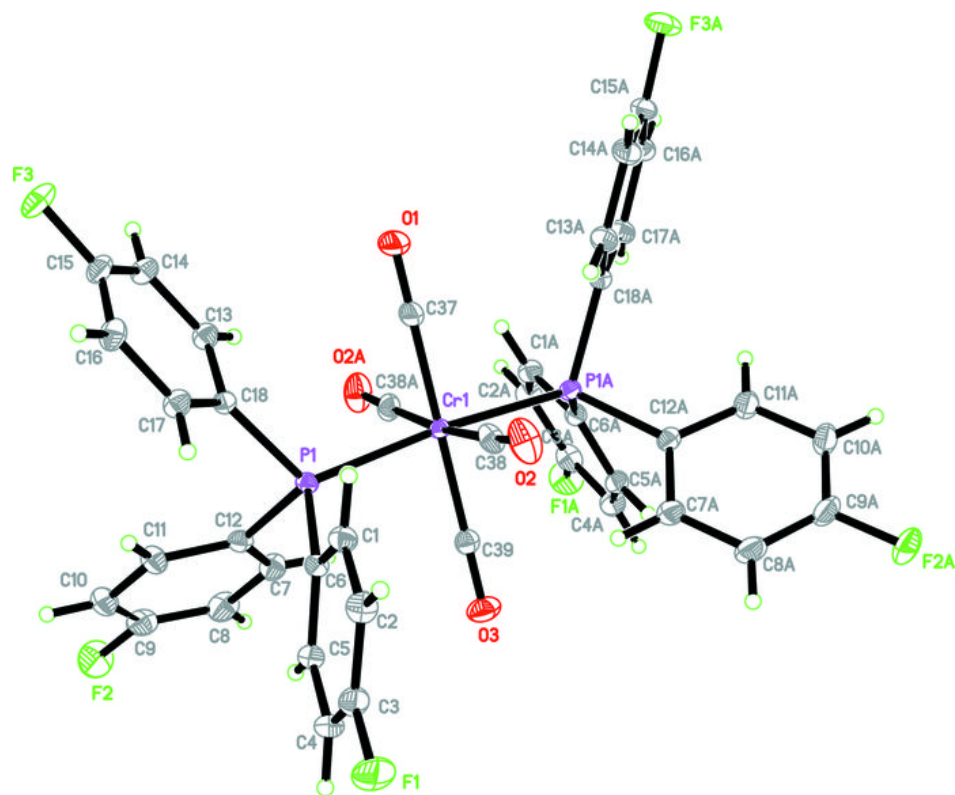


Fig. 2

