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Tricarbonyl(η^6-fluorobenzene)chromium

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Key indicators

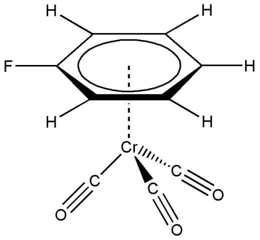
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.025
wR factor = 0.070
Data-to-parameter ratio = 14.9

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

The title compound, $[Cr(C_6H_5F)(CO)_3]$, exhibits the three-legged piano stool structure expected for a metal tricarbonyl complex with a η^6-coordinated arene. The fluoro functional group is tipped away from the $Cr(CO)_3$ center.

Comment

In the course of our work on the preparation and structure–property relationships of substituted organometallic compounds having arenes coordinated to chromium carbonyls, we isolated and structurally characterized the title compound, (I).



(I)

Compound (I) crystallizes in the monoclinic space group $P2_1/c$, with Z = 4 (Fig. 1 and Table 1). The fluoro functional group is displaced out of the least-squares plane defined by the atoms C1, C2, C3, C4, C5 and C6. The F atom and its *ipso* C atom, C1, are bent by 0.0082 (17) and 0.0100 (8) Å, respectively, away from the Cr atom. This distortion is consistent with our earlier structure–property relationship study of (η^6-arene)chromium(tricarbonyl) complexes (Hunter, Shilliday *et al.*, 1992), which revealed that π-donor groups on the arene bend away from the chromium fragments while π-accepting

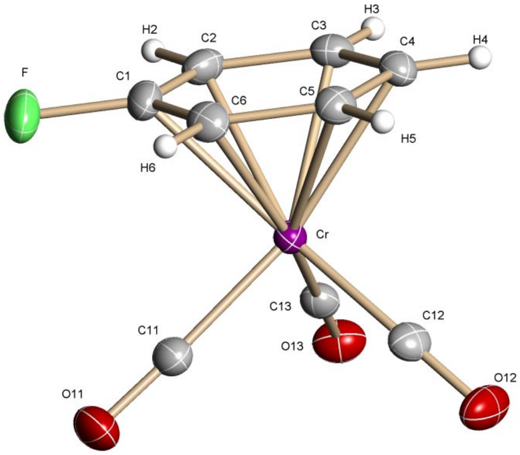


Figure 1
View of (I), showing 50% probability displacement ellipsoids.

groups remain in the plane of the arene or are bent slightly towards the chromium(tricarbonyl) fragments. The degree of bending was shown to be strongly correlated with the π-donor/acceptor strength of the substituents (Hunter, Mozol & Tsai, 1992). It is therefore not surprising that the observed structural distortion for this F substituent is similar to that reported for the OMe group, another moderately strong π-donor (Hunter, Mozol & Tsai, 1992), in (anisole)Cr(CO)$_3$ (Hunter, Shilliday *et al.*, 1992).

Experimental

The title compound was prepared from chromium(0) hexacarbonyl and fluorobenzene in a tetrahydrofuran/dibutyl ether mixture, as described previously (Hunter *et al.*, 1998). Pale-yellow single crystals of (I) were grown by the slow diffusion of a layer of hexane into a methylene chloride solution.

Crystal data

$[Cr(C_6H_5F)(CO)_3]$
$M_r = 232.13$
Monoclinic, $P2_1/c$
$a = 6.4048$ (8) Å
$b = 11.0668$ (14) Å
$c = 12.7124$ (16) Å
$\beta = 102.940$ (2)°
$V = 878.18$ (19) Å^3
$Z = 4$

$D_x = 1.756$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7097 reflections
$\theta = 2.5$–28.3°
$\mu = 1.29$ mm^{-1}
$T = 100$ (2) K
Block, yellow
0.46 × 0.28 × 0.23 mm

Data collection

Bruker *P*4 diffractometer
ω scans
Absorption correction: multi-scan (*SADABS* in *SAINT-Plus*; Bruker, 1997–1999)
$T_{min} = 0.542$, $T_{max} = 0.743$
8984 measured reflections

2190 independent reflections
2067 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 28.3°$
$h = -8 \rightarrow 8$
$k = -14 \rightarrow 14$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.070$
$S = 1.08$
2190 reflections
147 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 0.2388P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cr—C11	1.8441 (12)	O11—C11	1.1495 (15)
Cr—C12	1.8442 (12)	O12—C12	1.1534 (15)
Cr—C13	1.8493 (12)	O13—C13	1.1521 (15)
Cr—C5	2.2151 (12)	C1—C2	1.3908 (18)
Cr—C1	2.2151 (12)	C1—C6	1.406 (2)
Cr—C3	2.2198 (12)	C2—C3	1.4191 (17)
Cr—C6	2.2221 (12)	C3—C4	1.4015 (17)
Cr—C4	2.2292 (12)	C4—C5	1.4154 (16)
Cr—C2	2.2343 (12)	C5—C6	1.4047 (17)
F—C1	1.3442 (14)		
C11—Cr—C12	90.44 (6)	C4—C3—C2	120.69 (11)
C11—Cr—C13	88.44 (5)	C3—C4—C5	119.73 (10)
C12—Cr—C13	87.51 (5)	C6—C5—C4	120.42 (11)
F—C1—C2	118.55 (11)	C5—C6—C1	118.24 (10)
F—C1—C6	118.51 (11)	O11—C11—Cr	177.82 (12)
C2—C1—C6	122.92 (11)	O12—C12—Cr	179.12 (11)
C1—C2—C3	117.97 (11)	O13—C13—Cr	179.07 (10)

All H atoms were located in an electron difference map and were refined isotropically [C—H = 0.898 (16)–1.030 (15) Å]. The s.u. values of the cell parameters are taken from the software, recognizing that the values are unreasonably small (Herbstein, 2000).

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

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