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Tricarbonyl(η^6-trifluoromethylbenzene)-chromium(0)

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The title compound, $[Cr(C_6H_5CF_3)(CO)_3]$, exhibits the three-legged piano-stool structure expected for a tricarbonylmetal complex with an η^6-coordinated arene. The trifluoromethyl functional group is tilted towards the $Cr(CO)_3$ center.

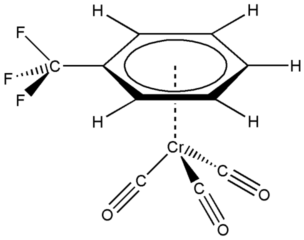
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.029
wR factor = 0.081
Data-to-parameter ratio = 14.6

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

Comment

In the course of our work on the preparation and property exploration of substituted arenes coordinated to chromium carbonyls, we isolated and structurally characterized the title compound, (I).



(I)

Compound (I) crystallizes in the monoclinic space group $P2_1/n$ with Z = 4 (Fig. 1 and Table 1). The trifluoromethyl functional group is tilted out of the least squares plane defined by the atoms C1/C2/C3/C4/C5/C6. The trifluoromethyl atom C7 is bent by 0.024 (4) Å towards the Cr atom. This distortion is consistent with an earlier structure–property relationship study of (η^6-arene)tricarbonylchromium complexes (Hunter, Shilliday *et al.*, 1992), which revealed that π-accepting groups on the arene remain in the plane of the arene or are bent slightly towards the tricarbonylchromium fragments while π-donor substituents bend away from the chromium 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 CF_3 derivative is similar to that observed for other moderately strong π-accepting substituents such as $SiMe_3$, C(O)Me, and CO_2Me (Hunter, Shilliday *et al.*, 1992, and references therein).

Experimental

The title compound, (I), was prepared from hexacarbonylchromium(0) and trifluoromethylbenzene in dibutyl ether 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

$[Cr(C_7H_5F_3)(CO)_3]$
$M_r = 282.14$
Monoclinic, $P2_1/n$
$a = 6.401$ (2) Å
$b = 11.500$ (4) Å
$c = 13.932$ (4) Å
$\beta = 91.908$ (5)°
$V = 1024.9$ (6) Å^3
$Z = 4$
$D_x = 1.828$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7855 reflections
$\theta = 2.3$–28.3°
$\mu = 1.15$ mm^{-1}
$T = 100$ (2) K
Plate, yellow
0.60 × 0.42 × 0.14 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi scan (*SADABS* in *SAINT-Plus*; Bruker, 1997–1999)
$T_{min} = 0.568$, $T_{max} = 0.851$
9901 measured reflections
2532 independent reflections
2328 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 28.3°$
$h = -8 \rightarrow 8$
$k = -15 \rightarrow 15$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.081$
$S = 1.09$
2532 reflections
174 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.044P)^2 + 0.3633P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.55$ e Å^{-3}
$\Delta\rho_{min} = -0.31$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cr—C13	1.8513 (16)	F3—C7	1.3372 (19)
Cr—C12	1.8560 (15)	C1—C6	1.404 (2)
Cr—C11	1.8588 (16)	C1—C2	1.416 (2)
Cr—C1	2.1867 (15)	C1—C7	1.502 (2)
Cr—C6	2.1898 (16)	C2—C3	1.404 (2)
Cr—C2	2.2154 (15)	C3—C4	1.420 (2)
Cr—C4	2.2177 (16)	C4—C5	1.397 (2)
Cr—C5	2.2203 (16)	C5—C6	1.420 (2)
Cr—C3	2.2238 (16)	C11—O11	1.146 (2)
F1—C7	1.336 (2)	C12—O12	1.1478 (18)
F2—C7	1.336 (2)	C13—O13	1.1527 (19)
C13—Cr—C12	88.40 (7)	C1—C6—C5	119.95 (14)
C13—Cr—C11	88.67 (7)	F2—C7—F1	106.95 (13)
C12—Cr—C11	89.12 (7)	F2—C7—F3	106.80 (14)
C6—C1—C2	120.20 (13)	F1—C7—F3	106.93 (13)
C6—C1—C7	119.31 (13)	F2—C7—C1	112.26 (13)
C2—C1—C7	120.49 (13)	F1—C7—C1	111.37 (14)
C3—C2—C1	119.82 (13)	F3—C7—C1	112.19 (13)
C2—C3—C4	119.86 (14)	O11—C11—Cr	178.77 (14)
C5—C4—C3	120.37 (14)	O12—C12—Cr	179.71 (14)
C4—C5—C6	119.77 (13)	O13—C13—Cr	178.99 (13)

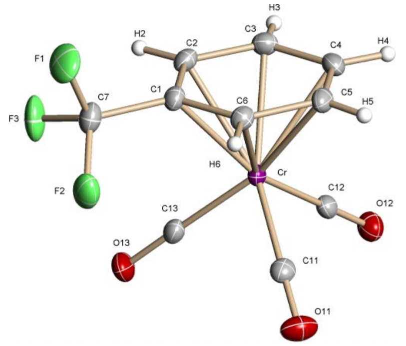


Figure 1
View of (I), showing 50% probability displacement ellipsoids.

All H atoms were located in an electron difference map and were refined isotropically. 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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