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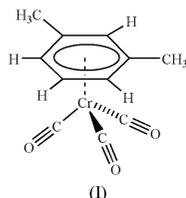
Key indicators

Single-crystal X-ray study
T = 100 K
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
R factor = 0.032
wR factor = 0.083
Data-to-parameter ratio = 16.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Tricarbonyl(η^6 -1,3-dimethylbenzene)chromium

The title compound, $[\text{Cr}(1,3\text{-Me}_2\text{C}_6\text{H}_4)(\text{CO})_3]$, exhibits the three-legged piano stool structure expected for a metal tricarbonyl with an η^6 -coordinated arene. The compound displays mirror symmetry in the solid state.

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). It crystallizes in the monoclinic space group $P2_1/m$, with two molecules in the unit cell. The molecule exhibits a crystallographic mirror plane (Fig. 1 and Table 1) that bisects the benzene ring and passes through the Cr atom and one of the carbonyl groups.



The methyl groups are slightly bent out of the C3/C4/C5/C6/C5ⁱ/C4ⁱ least-squares plane, towards the Cr atom, with an r.m.s. deviation of 0.012 (3) Å [symmetry code: (i) $x, \frac{3}{2} - y, z$]. This distortion is consistent with that reported by an earlier structure–property relationship study of (η^6 -arene)-chromium(tricarbonyl) complexes (Hunter *et al.*, 1992). This study revealed that π -donor substituents on the arene bend away from the chromium(tricarbonyl) fragments, while π -accepting or ‘innocent’ groups like methyl remain in the plane of the arene or are bent slightly towards the chromium fragment, the degree of bending being correlated with the π -donor/acceptor strength of the substituents.

Experimental

Compound (I) was prepared from chromium(0) hexacarbonyl and 1,3-dimethylbenzene in a mixture of dibutyl ether and tetrahydrofuran as previously described (Hunter *et al.*, 1992). Pale-yellow single crystals of (I) were grown by the slow diffusion of a layer of hexane into a methylene chloride solution.

Crystal data

$[\text{Cr}(\text{C}_8\text{H}_{10})(\text{CO})_3]$
 $M_r = 242.19$
 Monoclinic, $P2_1/m$
 $a = 6.0907$ (5) Å
 $b = 12.8263$ (10) Å
 $c = 6.7722$ (6) Å
 $\beta = 100.029$ (1)°
 $V = 520.97$ (7) Å³
 $Z = 2$

$D_x = 1.544 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 3836
 reflections
 $\theta = 3.1\text{--}28.1^\circ$
 $\mu = 1.08 \text{ mm}^{-1}$
 $T = 100$ (2) K
 Block, yellow
 $0.22 \times 0.11 \times 0.05 \text{ mm}$

Data collection

Bruker SMART APEX
diffractometer
 ω scans
Absorption correction: multi-scan
(*SADABS* in *SAINT-Plus*;
Bruker, 1997–1999)
 $T_{\min} = 0.799$, $T_{\max} = 0.950$
4449 measured reflections

1252 independent reflections
1168 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$
 $\theta_{\text{max}} = 28.2^\circ$
 $h = -7 \rightarrow 8$
 $k = -16 \rightarrow 16$
 $l = -8 \rightarrow 8$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.083$
 $S = 1.12$
1252 reflections
77 parameters
All H-atom parameters refined

$w = 1/[\sigma^2(F_o^2) + (0.0386P)^2 + 0.4125P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.56 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.25 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Cr1–C8	1.832 (2)	O1–C7	1.141 (4)
Cr1–C7	1.845 (3)	O2–C8	1.154 (3)
Cr1–C3	2.199 (3)	C2–C5	1.506 (3)
Cr1–C4	2.2244 (19)	C3–C4	1.399 (2)
Cr1–C6	2.226 (3)	C4–C5	1.407 (3)
Cr1–C5	2.2332 (19)	C5–C6	1.409 (3)
C8^i –Cr1–C8	86.98 (12)	C4–C5–C2	120.0 (2)
C8–Cr1–C7	89.67 (9)	C6–C5–C2	121.5 (2)
C4^i –C3–C4	121.7 (2)	C5–C6–C5 ⁱ	122.1 (2)
C3–C4–C5	119.64 (19)	O1–C7–Cr1	179.1 (3)
C4–C5–C6	118.50 (19)	O2–C8–Cr1	178.39 (17)

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

All H atoms were located in a difference density map and refined isotropically [$\text{C–H} = 0.89$ (4)– 0.99 (3) \AA]. 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*;

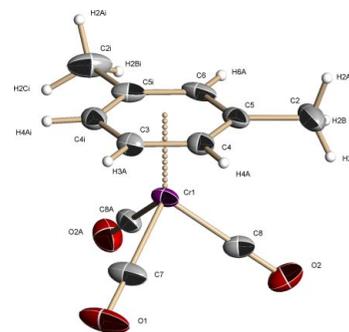


Figure 1

The molecular structure of (I), showing 30% probability displacement ellipsoids. [Symmetry code: $A \ x, \frac{3}{2} - y, z$.]

program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXL97*.

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