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## Key indicators

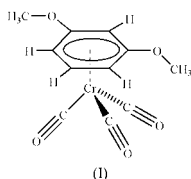
Single-crystal X-ray study  
 $T = 273$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å  
 $R$  factor = 0.031  
 $wR$  factor = 0.089  
Data-to-parameter ratio = 12.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.Tricarbonyl( $\eta^6$ -1,3-dimethoxybenzene)chromium

The title compound,  $[\text{Cr}\{1,3-(\text{MeO})_2\text{C}_6\text{H}_4\}(\text{CO})_3]$ , exhibits the three-legged piano stool structure expected for a metal tricarbonyl with an  $\eta^6$ -coordinated arene. Two independent mirror-symmetric molecules are found in the unit cell. The methoxy groups display an out-of-plane distortion.

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## 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 orthorhombic space group  $Pnma$ , with  $Z = 8$  and two independent molecules in the unit cell. Each molecule exhibits a crystallographic mirror plane (Fig. 1 and Table 1), bisecting the benzene rings and passing through the Cr atom and one of the carbonyl groups.



The methoxy functional groups are distorted out of the  $\text{C}1-\text{C}4/\text{C}3^i/\text{C}2^i$  and  $\text{C}1'-\text{C}4'/\text{C}3'^i/\text{C}2'^i$  least-squares planes [symmetry code: (i)  $x, \frac{1}{2} - y, z$ ]. The methoxy groups are bent by 0.054 (3) and 0.061 (3) Å away from the Cr atoms. This distortion is consistent with that reported for an earlier structure–property relationship study of ( $\eta^6$ -arene)-chromium(tricarbonyl) complexes (Hunter *et al.*, 1992). This study revealed that  $\pi$ -donor substituents on the arene bend away from the chromium(tricarbonyl) fragments, while  $\pi$ -accepting groups remain in the plane of the arene or are bent slightly towards the chromium fragment, the degree of bending being correlated with the  $\pi$ -donor/acceptor strength of the substituents.

## Experimental

The title compound, (I), was prepared from chromium(0) hexacarbonyl and 1,3-dimethoxybenzene 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

$[\text{Cr}(\text{C}_8\text{H}_{10}\text{O}_2)(\text{CO})_3]$   
 $M_r = 274.19$   
Orthorhombic,  $Pnma$   
 $a = 11.5948$  (19) Å  
 $b = 13.440$  (2) Å  
 $c = 13.046$  (2) Å  
 $V = 2033.0$  (6) Å<sup>3</sup>  
 $Z = 8$   
 $D_x = 1.792$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
Cell parameters from 6108  
reflections  
 $\theta = 2.2$ – $28.1^\circ$   
 $\mu = 1.13$  mm<sup>-1</sup>  
 $T = 273$  (2) K  
Plate, yellow  
 $0.82 \times 0.16 \times 0.02$  mm

## Data collection

Bruker AXS SMART APEX CCD  
diffractometer

$\omega$  scans

Absorption correction: multi-scan  
(*SADABS* in *SAINT-Plus*;  
Bruker, 1997–1999)

$T_{\min} = 0.779$ ,  $T_{\max} = 0.980$

12 064 measured reflections

2549 independent reflections

1983 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\text{max}} = 28.2^\circ$

$h = -15 \rightarrow 15$

$k = -17 \rightarrow 17$

$l = -17 \rightarrow 11$

## Refinement

Refinement on  $F^2$

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.089$

$S = 1.04$

2549 reflections

213 parameters

Only coordinates of H atoms  
refined

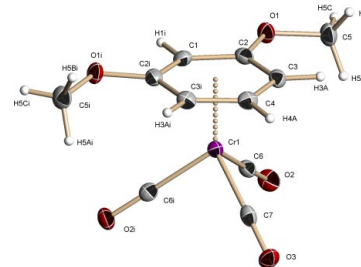
$w = 1/[\sigma^2(F_o^2) + (0.0454P)^2 + 1.1678P]$

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

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.41 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.46 \text{ e } \text{\AA}^{-3}$



**Figure 1**

The molecular structure of one of the independent molecules of (I), showing 30% probability displacement ellipsoids. [Symmetry code: (i)  $x, \frac{1}{2} - y, z$ .]

Data collection: *SMART* (Bruker, 1997–2000); cell refinement: *SAINT-Plus* (Bruker, 1997–1999); data reduction: *SAINT-Plus*; 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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**Table 1**

Selected geometric parameters (Å).

Cr2–C7'	1.784 (3)	Cr1–C7	1.786 (3)
Cr2–C6'	1.789 (2)	Cr1–C6	1.792 (2)
Cr2–C4'	2.135 (3)	Cr1–C4	2.123 (3)
Cr2–C1'	2.184 (3)	Cr1–C3	2.181 (2)
Cr2–C3'	2.184 (2)	Cr1–C1	2.200 (3)
Cr2–C2'	2.217 (2)	Cr1–C2	2.231 (2)
O1'–C2'	1.316 (2)	O3–C7	1.131 (4)
O1'–C5'	1.403 (2)	O1–C2	1.314 (2)
O3'–C7'	1.129 (4)	O1–C5	1.404 (2)
O2'–C6'	1.129 (3)	O2–C6	1.126 (2)
C1'–C2'	1.375 (2)	C4–C3	1.369 (3)
C3'–C4'	1.370 (3)	C1–C2	1.370 (2)
C3'–C2'	1.371 (3)	C2–C3	1.374 (3)

All H atoms were located in difference Fourier maps and their positional parameters were refined, with  $U_{\text{iso}}$  defined as  $1.2U_{\text{eq}}$  or  $1.5U_{\text{eq}}$  of the parent atom. The C–H bond lengths are 0.87 (4)–0.98 (4) Å. The s.u. values of the cell parameters are taken from the software, recognizing that the values are unreasonably small (Herbstein, 2000).