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Key indicators

Single-crystal X-ray study
 $T = 110$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.033
 wR factor = 0.084
Data-to-parameter ratio = 22.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Tricarbonyl $\{\eta^6-(S,S)$ -1-[2-methoxy-3,6-bis(trimethylsilyl)phenyl]- N,N -dimethylethylamine $\}$ -chromium(0)

The title complex, $[\text{Cr}(\text{C}_{17}\text{H}_{33}\text{NOSi}_2)(\text{CO})_3]$, has the typical three-legged piano-stool structure expected for η^6 -arenetricarbonylchromium compounds. The conformation is staggered with respect to the methoxy group of the arene ring and one of the carbonyl ligands.

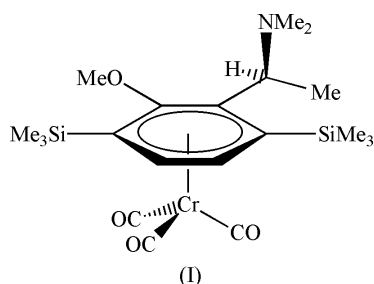
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Comment

In the course of our work (Totev *et al.*, 2004; Braun *et al.*, 2004; Englert *et al.*, 2004; Salzer, 2003) on the diastereoselective synthesis of planar chiral arenetricarbonylchromium complexes, we synthesized and structurally characterized the title complex, (I) (Fig. 1). The complex crystallizes in the non-centrosymmetric orthorhombic space group $P2_12_12_1$.



The non-H atoms attached to the complexed arene ring are displaced from the least-squares plane defined by the atoms in the aromatic ring (C104–C109) to various extents; a considerable distortion of -0.193 (1) Å (towards the Cr atom) is observed for Si1, whereas Si2 shows a displacement of only

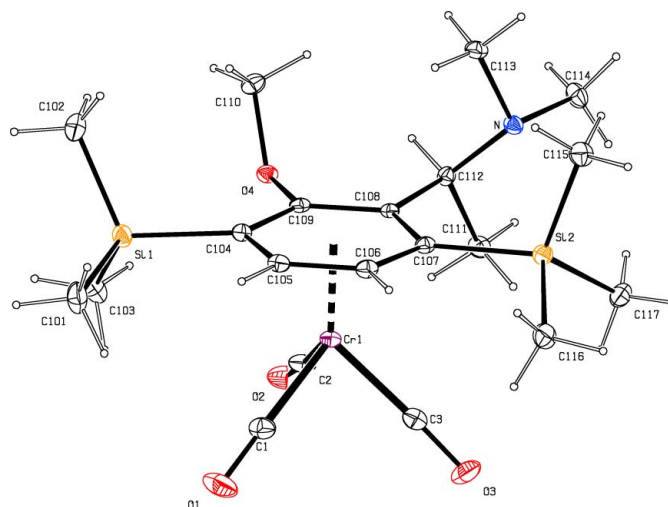


Figure 1
View of (I), with 30% displacement ellipsoids and H atoms shown as spheres of arbitrary radii.

0.068 (1) Å (away from the Cr atom). Atom C112 is displaced by 0.088 (2) Å and O1 shows the smallest displacement of -0.006 (1) Å. The N—C112—C108—C107 torsion angle is 133.5 (2)°. The lone pair of electrons of the N atom of the chiral side chain point towards the adjacent trimethylsilyl group [N⋯Si2 = 3.059 (3) Å], while the two *N*-methyl groups are pointing away from Si2 to minimize steric hindrance.

Experimental

Compound (I) was synthesized by thermal complexation of (*S,S*)-1-[2-methoxy-3,6-bis(trimethylsilyl)phenyl]-*N,N*-dimethylethylamine using Kündig's reagent (naphthalene)Cr(CO)₃ (Kündig *et al.*, 1985) in a high-pressure Schlenk tube in an *n*-Bu₂O/tetrahydrofuran mixture. After work-up, yellow single crystals were obtained by slow diffusion of hexanes into a diethyl ether solution at 243 K.

Crystal data

[Cr(C ₁₇ H ₃₃ NOSi ₂)(CO) ₃]	Mo K α radiation
$M_r = 459.65$	Cell parameters from 8096 reflections
Orthorhombic, $P2_12_12_1$	$\theta = 1.6\text{--}28.3^\circ$
$a = 7.1361$ (12) Å	$\mu = 0.60$ mm ⁻¹
$b = 17.251$ (3) Å	$T = 110$ (2) K
$c = 19.541$ (3) Å	Rod, yellow
$V = 2405.7$ (7) Å ³	$0.44 \times 0.03 \times 0.03$ mm
$Z = 4$	
$D_x = 1.269$ Mg m ⁻³	

Data collection

Bruker SMART APEX CCD diffractometer	5984 independent reflections
ω scans	5037 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.071$
$T_{\text{min}} = 0.779$, $T_{\text{max}} = 0.982$	$\theta_{\text{max}} = 28.3^\circ$
33 064 measured reflections	$h = -9 \rightarrow 9$
	$k = -22 \rightarrow 22$
	$l = -26 \rightarrow 26$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0411P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.033$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.084$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 0.92$	$\Delta\rho_{\text{max}} = 0.38$ e Å ⁻³
5984 reflections	$\Delta\rho_{\text{min}} = -0.28$ e Å ⁻³
263 parameters	Absolute structure: Flack (1983),
H-atom parameters constrained	2578 Friedel pairs
	Flack parameter = -0.006 (18)

Table 1

Selected geometric parameters (Å, °).

Cr1—C3	1.844 (3)	Cr1—C106	2.236 (2)
Cr1—C2	1.846 (3)	Cr1—C104	2.246 (2)
Cr1—C1	1.850 (3)	Cr1—C107	2.270 (2)
Cr1—C105	2.214 (3)	Cr1—C108	2.272 (2)
Cr1—C109	2.235 (2)		
C3—Cr1—C2	88.76 (12)	C2—Cr1—C1	87.98 (12)
C3—Cr1—C1	85.17 (12)		

H atoms were placed in calculated positions, with C—H = 0.98 Å, and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.3U_{\text{eq}}(\text{C})$. Methyl groups were allowed to rotate as rigid groups.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT-Plus (Bruker, 1999); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

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