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Bis(η^5-1,3-di-*tert*-butylcyclopentadienyl)-chromium(II)

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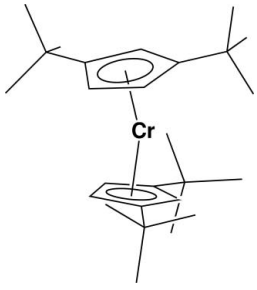
Key indicators: single-crystal X-ray study; T = 134 K; mean σ(C–C) = 0.004 Å; R factor = 0.043; wR factor = 0.114; data-to-parameter ratio = 17.1.

The title compound, $[Cr(C_{13}H_{21})_2]$ or $[\eta^5\text{-}1,3\text{-}(Me_3C)_2C_5H_3]_2Cr$, a substituted chromocene, crystallizes with two independent half-molecules in the asymmetric unit, the molecules having twofold rotation symmetry. The compound is isostructural with the iron and cobalt analogues and is a bent metallocene.

Related literature

The corresponding iron and cobalt metallocenes are isostructural (Boese *et al.*, 1993; Schneider *et al.*, 1997). Five other chromocenes have been structurally characterized (Flower & Hitchcock, 1996; Castellani *et al.*, 1987; Overby *et al.*, 1998; Blümel *et al.*, 1996; Benetollo *et al.*, 1994). For related literature, see: Schultz *et al.* (2000, 2001).



Experimental

Crystal data

$[Cr(C_{13}H_{21})_2]$
M_r = 406.60
Orthorhombic, *Pccn*
a = 11.7750 (6) Å
b = 12.4122 (6) Å
c = 32.621 (2) Å
V = 4767.7 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.49 mm^{-1}
T = 134 (2) K
0.21 × 0.19 × 0.08 mm

Data collection

Bruker SMART 1K CCD diffractometer
Absorption correction: multi-scan (*XPREP*; Sheldrick, 1995)
T_{min} = 0.905, T_{max} = 0.962
21800 measured reflections
4385 independent reflections
2665 reflections with $I > 2\sigma(I)$
R_{int} = 0.077

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.114
S = 1.02
4385 reflections
257 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cr1—C1	2.180 (3)	Cr2—C6	2.224 (3)
Cr1—C2	2.225 (3)	Cr2—C7	2.230 (3)
Cr1—C3	2.228 (3)	Cr2—C8	2.179 (3)
Cr1—C4	2.133 (3)	Cr2—C9	2.104 (3)
Cr1—C5	2.111 (3)	Cr2—C10	2.128 (3)
Cr1—*Cg*1	1.807	Cr2—*Cg*2	1.805
*Cg*1^{i}—Cr1—*Cg*1	173.3	*Cg*2^{ii}—Cr2—*Cg*2	173.1

Symmetry codes: (i) $-x+\frac{1}{2}, -y+\frac{3}{2}, z$; (ii) $-x+\frac{1}{2}, -y+\frac{1}{2}, z$. *Cg*1 and *Cg*2 are the centroids of the rings C1–C5 and C6–C10, respectively.

Data collection: *SMART* (Siemens, 1995); cell refinement: *SAINT* (Siemens, 1995); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 1998); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SG2205).

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supplementary materials

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Bis(η^5-1,3-di-*tert*-butylcyclopentadienyl)chromium(II)

M. Schultz

Comment

The properties of metallocenes vary widely depending on the substituents on the cyclopentadienyl ring. The bulky ligand $[1,3\text{-}(Me_3C)_2C_5H_3]^-$ has been found to have electronic properties similar to $(Me_5C_5)^-$ in ytterbocenes (Schultz *et al.*, 2001), but quite different steric properties leading to different solid state packing arrangements in the base-free metallocenes (Schultz *et al.*, 2000). The chromocene of this ligand, the title compound (I), was prepared as part of a study of first row metallocenes with bulky substituents.

The compound (I) crystallizes with two half-molecules in the asymmetric unit and the metals lying on special positions. The compound is isostructural with the iron and cobalt analogues, which are the only other base-free transition metal metallocenes with this ligand that have been structurally characterized (Boese *et al.*, 1993), (Schneider *et al.*, 1997). Table 1 gives selected bond distances and angles for (I); *Cg*1 and *Cg*2 are the calculated centroids of the rings C1 - C5 and C6 - C10, respectively. Figure 1 is an *ORTEP* diagram showing the atom labelling scheme.

Compound (I) is the first example of a bent chromocene, with centroid - metal - centroid angle 173°. The metallocenes $[1,3\text{-}(Me_3C)_2C_5H_3]_2Fe$ and $[1,3\text{-}(Me_3C)_2C_5H_3]_2Co$ are also unusual examples of bent metallocenes of those metals. This is presumably due to the steric bulk of the four tertiary butyl groups, which force the rings to bend back although there are no close metal - carbon distances indicating agostic metal - hydrogen interactions.

The twist angle of a metallocene is defined as the mean value of the five angles between a ring carbon atom on the upper ring and the closest one on the lower ring. The angles are measured between the planes defined by the two centroids and each ring carbon atom. Thus, it can vary from zero (perfectly eclipsed), in which the rings lie directly above one another, to 36° (completely staggered), in which the plane containing the lower carbon atom bisects the 72° angle between two carbon atoms of the upper ring. The cyclopentadienyl rings of the two unique molecules in (I) are close to being eclipsed (twist angle molecule 1: 14.4°; molecule 2: 13.2°) and are oriented so that the tertiary butyl groups lie on alternating positions on each ring, presumably to minimize steric repulsions.

It is informative to compare the structural parameters for (I) with those of the five other base-free chromium(II) metallocenes that have been structurally characterized (excluding *ansa*-bridged examples). In the structures of unsubstituted $(C_5H_5)_2Cr$ (Flower & Hitchcock, 1996), $(1,2,3,4\text{-}Ph_4C_5H)_2Cr$ (Castellani *et al.*, 1987) and $[1,2,4\text{-}(Me_2CH)_3C_5H_2]_2Cr$ (Overby *et al.*, 1998), the chromium metal lies on a crystallographic inversion centre and the cyclopentadienyl rings are therefore exactly parallel and perfectly staggered (twist angles 36°). In $(Me_5C_5)_2Cr$ (Blümel *et al.*, 1996) and $(MeC_5H_4)_2Cr$ (Benetollo *et al.*, 1994), the centroid-metal-centroid angles are 179/180° (two unique molecules) and 178°, respectively, and the twist angles are 17/7° and 3°. Thus, (I) is the only significantly bent chromocene, although the twist angles in (I) are not unusual. The metal - ring centroid distances in all of these structures lie between 1.78 and 1.81 Å, except for $(1,2,3,4\text{-}Ph_4C_5H)_2Cr$ (1.832 Å), which shows elongated metal - ring distances due to the extreme bulk of the ligand in that case.

Experimental

The sodium salt Na[1,3-$(Me_3C)_2C_5H_3$] (2.71 g, 0.0135 mol) and $Cr_2(OAc)_4$ (1.15 g, 3.39 mmol) were weighed into a Schlenk flask equipped with a magnetic stirrer under a flow of dinitrogen. THF (180 ml) was added and the slurry was stirred at room temperature for one hour, then heated to reflux and stirred at reflux overnight. The solvent was then removed under reduced pressure and the residue was extracted to pentane (100 ml). The volume of solvent was reduced and the solution was cooled to −80°C. Large red air-sensitive crystals formed in 77% yield. mp 183–184°C. ^{1}H NMR (C_6D_6, 23°C): δ 0.2 ($\nu_{1/2}$ = 250 Hz, Me_3C) (ring protons not observed). The molecule sublimes under dynamic vacuum. The synthesis of compound (I) has also been reported by a different route (Overby *et al.*, 1998). For data collection, a red crystal was placed in Paratone N hydrocarbon oil and then mounted on a glass fiber.

Figures

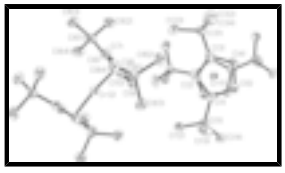


Fig. 1. A view of the two independent molecules of (I) showing the atom labelling scheme for one ring of each molecule (the second ring on each molecule is generated by symmetry). Hydrogen atoms have been omitted for clarity. Displacement ellipsoids are drawn at the 50% probability level.

Bis(η^5-1,3-di-*tert*-butylcyclopentadienyl)chromium(II)

Crystal data

$[Cr(C_{13}H_{21})_2]$	D_x = 1.133 Mg m^{-3}
M_r = 406.60	Melting point: not measured K
Orthorhombic, *Pccn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ab 2ac	Cell parameters from 5151 reflections
a = 11.7750 (6) Å	θ = 1.5–44.3º
b = 12.4122 (6) Å	μ = 0.49 mm^{-1}
c = 32.621 (2) Å	*T* = 134 (2) K
V = 4767.7 (4) Å^3	Block, red
Z = 8	0.21 × 0.19 × 0.08 mm
F_{000} = 1776	

Data collection

Bruker SMART 1K CCD diffractometer	4385 independent reflections
Radiation source: fine-focus sealed tube	2665 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.077
T = 134(2) K	θ_{max} = 26.3º
ω–scan	θ_{min} = 1.3º
Absorption correction: multi-scan (XPREP; Sheldrick, 1995)	*h* = −12→13

T_{min} = 0.905, T_{max} = 0.962
21800 measured reflections
k = −14→15
l = −29→39

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.114
S = 1.02
4385 reflections
257 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 1.131P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Extinction correction: none

Special details

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cr1	0.2500	0.7500	0.044372 (18)	0.01940 (17)
Cr2	0.2500	0.2500	0.181375 (18)	0.01916 (17)
C1	0.3177 (2)	0.5946 (2)	0.02512 (9)	0.0212 (7)
C2	0.3437 (2)	0.6067 (2)	0.06750 (8)	0.0207 (7)
H2	0.3188	0.5594	0.0886	0.025*
C3	0.4122 (2)	0.6995 (2)	0.07379 (8)	0.0222 (7)
C4	0.4290 (2)	0.7466 (2)	0.03457 (8)	0.0234 (6)
H4	0.4712	0.8102	0.0292	0.028*
C5	0.3721 (2)	0.6824 (2)	0.00459 (9)	0.0220 (7)
H5	0.3706	0.6957	−0.0241	0.026*
C6	0.2885 (2)	0.4079 (2)	0.21043 (9)	0.0228 (7)
C7	0.3923 (2)	0.3517 (2)	0.20460 (9)	0.0230 (7)
H7	0.4439	0.3332	0.2259	0.028*
C8	0.4079 (2)	0.3272 (2)	0.16259 (9)	0.0213 (7)
C9	0.3112 (2)	0.3702 (2)	0.14162 (9)	0.0221 (7)
H9	0.2981	0.3669	0.1129	0.026*
C10	0.2378 (3)	0.4189 (2)	0.17099 (9)	0.0252 (7)
H10	0.1673	0.4528	0.1653	0.030*
C11	0.2585 (3)	0.4994 (2)	0.00510 (8)	0.0239 (6)
C12	0.1652 (3)	0.4525 (2)	0.03243 (9)	0.0309 (8)

H12A	0.1978	0.4315	0.0589	0.046*
H12B	0.1320	0.3892	0.0191	0.046*
H12C	0.1061	0.5069	0.0368	0.046*
C13	0.3488 (3)	0.4123 (2)	−0.00243 (11)	0.0428 (9)
H13A	0.4074	0.4406	−0.0208	0.064*
H13B	0.3131	0.3491	−0.0150	0.064*
H13C	0.3834	0.3916	0.0237	0.064*
C14	0.2046 (3)	0.5316 (3)	−0.03600 (9)	0.0365 (8)
H14A	0.1471	0.5873	−0.0313	0.055*
H14B	0.1688	0.4684	−0.0485	0.055*
H14C	0.2635	0.5596	−0.0544	0.055*
C61	0.2435 (3)	0.4578 (2)	0.25000 (9)	0.0271 (7)
C62	0.2590 (3)	0.5806 (2)	0.24669 (10)	0.0371 (8)
H62A	0.3396	0.5972	0.2426	0.056*
H62B	0.2322	0.6149	0.2720	0.056*
H62C	0.2151	0.6078	0.2234	0.056*
C63	0.3097 (3)	0.4167 (3)	0.28684 (9)	0.0359 (8)
H63A	0.3036	0.3381	0.2883	0.054*
H63B	0.2784	0.4485	0.3119	0.054*
H63C	0.3897	0.4372	0.2841	0.054*
C64	0.1172 (3)	0.4333 (3)	0.25587 (10)	0.0394 (9)
H64A	0.0746	0.4592	0.2320	0.059*
H64B	0.0897	0.4697	0.2806	0.059*
H64C	0.1065	0.3554	0.2587	0.059*
C31	0.4666 (2)	0.7361 (2)	0.11388 (9)	0.0256 (7)
C32	0.4532 (3)	0.8584 (2)	0.11985 (10)	0.0368 (8)
H32A	0.4852	0.8962	0.0961	0.055*
H32B	0.4934	0.8806	0.1447	0.055*
H32C	0.3724	0.8762	0.1225	0.055*
C33	0.4152 (3)	0.6778 (3)	0.15074 (9)	0.0361 (8)
H33A	0.3334	0.6919	0.1519	0.054*
H33B	0.4511	0.7039	0.1760	0.054*
H33C	0.4282	0.6001	0.1480	0.054*
C34	0.5942 (3)	0.7094 (3)	0.11186 (10)	0.0371 (8)
H34A	0.6040	0.6326	0.1059	0.056*
H34B	0.6298	0.7266	0.1382	0.056*
H34C	0.6299	0.7522	0.0901	0.056*
C81	0.5135 (2)	0.2797 (2)	0.14232 (9)	0.0234 (7)
C82	0.5899 (3)	0.3743 (3)	0.12892 (10)	0.0350 (8)
H82A	0.6575	0.3461	0.1150	0.053*
H82B	0.6130	0.4157	0.1531	0.053*
H82C	0.5477	0.4211	0.1101	0.053*
C83	0.4825 (3)	0.2132 (2)	0.10470 (9)	0.0340 (8)
H83A	0.4345	0.1525	0.1130	0.051*
H83B	0.5519	0.1859	0.0918	0.051*
H83C	0.4411	0.2584	0.0851	0.051*
C84	0.5793 (2)	0.2087 (3)	0.17218 (9)	0.0316 (8)
H84A	0.5305	0.1497	0.1816	0.047*
H84B	0.6035	0.2518	0.1958	0.047*

H84C	0.6463	0.1789	0.1584	0.047*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.0175 (3)	0.0205 (3)	0.0202 (4)	0.0028 (3)	0.000	0.000
Cr2	0.0189 (3)	0.0191 (3)	0.0195 (3)	−0.0008 (3)	0.000	0.000
C1	0.0182 (16)	0.0217 (15)	0.0237 (17)	0.0048 (13)	0.0014 (13)	0.0011 (13)
C2	0.0205 (16)	0.0207 (15)	0.0208 (16)	0.0032 (13)	0.0000 (13)	0.0015 (13)
C3	0.0176 (15)	0.0264 (16)	0.0227 (17)	0.0032 (13)	−0.0001 (13)	0.0017 (14)
C4	0.0186 (14)	0.0208 (14)	0.0308 (16)	0.0001 (14)	0.0038 (12)	−0.0007 (15)
C5	0.0184 (15)	0.0250 (16)	0.0225 (17)	0.0041 (13)	0.0042 (13)	−0.0001 (13)
C6	0.0226 (15)	0.0218 (15)	0.0241 (17)	−0.0014 (13)	0.0007 (13)	0.0006 (13)
C7	0.0240 (16)	0.0239 (15)	0.0210 (17)	−0.0032 (13)	−0.0051 (13)	0.0025 (13)
C8	0.0215 (16)	0.0200 (15)	0.0225 (16)	−0.0054 (13)	−0.0012 (13)	0.0012 (13)
C9	0.0271 (17)	0.0194 (15)	0.0198 (17)	−0.0032 (13)	−0.0005 (13)	0.0033 (13)
C10	0.0241 (17)	0.0192 (14)	0.0322 (17)	0.0015 (14)	−0.0014 (14)	0.0025 (13)
C11	0.0256 (16)	0.0224 (14)	0.0236 (15)	0.0009 (14)	0.0006 (15)	−0.0023 (12)
C12	0.0351 (19)	0.0294 (17)	0.0281 (19)	−0.0065 (15)	−0.0056 (15)	0.0023 (15)
C13	0.039 (2)	0.0292 (18)	0.060 (2)	0.0042 (16)	−0.0033 (18)	−0.0139 (18)
C14	0.046 (2)	0.038 (2)	0.0246 (19)	−0.0098 (16)	−0.0054 (15)	−0.0028 (15)
C31	0.0210 (15)	0.0266 (17)	0.0292 (17)	0.0015 (14)	−0.0045 (13)	−0.0037 (14)
C32	0.039 (2)	0.0331 (19)	0.039 (2)	0.0012 (16)	−0.0122 (16)	−0.0095 (16)
C33	0.040 (2)	0.043 (2)	0.0256 (19)	−0.0033 (16)	−0.0072 (16)	0.0005 (16)
C34	0.0281 (18)	0.044 (2)	0.039 (2)	0.0013 (15)	−0.0122 (16)	−0.0042 (16)
C61	0.0242 (16)	0.0265 (16)	0.0306 (17)	−0.0005 (16)	0.0003 (16)	−0.0067 (13)
C62	0.044 (2)	0.0304 (17)	0.0374 (19)	−0.0014 (18)	0.0040 (17)	−0.0119 (15)
C63	0.0387 (19)	0.042 (2)	0.0271 (19)	0.0016 (17)	0.0016 (16)	−0.0069 (16)
C64	0.0309 (19)	0.049 (2)	0.038 (2)	−0.0016 (17)	0.0084 (16)	−0.0178 (17)
C81	0.0197 (15)	0.0263 (17)	0.0242 (17)	−0.0006 (12)	0.0026 (13)	−0.0008 (13)
C82	0.0292 (18)	0.0374 (19)	0.038 (2)	−0.0041 (15)	0.0093 (16)	0.0024 (16)
C83	0.0324 (18)	0.0415 (19)	0.0280 (18)	0.0009 (15)	0.0050 (15)	−0.0053 (15)
C84	0.0248 (17)	0.0380 (18)	0.0321 (19)	0.0036 (15)	0.0027 (15)	0.0003 (15)

Geometric parameters (Å, °)

Cr1—C1^{i}	2.180 (3)	C12—H12A	0.9800
Cr1—C1	2.180 (3)	C12—H12B	0.9800
Cr1—C2^{i}	2.225 (3)	C12—H12C	0.9800
Cr1—C2	2.225 (3)	C13—H13A	0.9800
Cr1—C3^{i}	2.228 (3)	C13—H13B	0.9800
Cr1—C3	2.228 (3)	C13—H13C	0.9800
Cr1—C4^{i}	2.133 (3)	C14—H14A	0.9800
Cr1—C4	2.133 (3)	C14—H14B	0.9800
Cr1—C5^{i}	2.111 (3)	C14—H14C	0.9800
Cr1—C5	2.111 (3)	C61—C63	1.520 (4)
Cr1—Cg1	1.807	C61—C64	1.529 (4)
Cr2—C6	2.224 (3)	C61—C62	1.539 (4)

Cr2—C6^{ii}	2.224 (3)	C62—H62A	0.9800
Cr2—C7	2.230 (3)	C62—H62B	0.9800
Cr2—C7^{ii}	2.230 (3)	C62—H62C	0.9800
Cr2—C8^{ii}	2.179 (3)	C63—H63A	0.9800
Cr2—C8	2.179 (3)	C63—H63B	0.9800
Cr2—C9^{ii}	2.104 (3)	C63—H63C	0.9800
Cr2—C9	2.104 (3)	C64—H64A	0.9800
Cr2—C10	2.128 (3)	C64—H64B	0.9800
Cr2—C10^{ii}	2.128 (3)	C64—H64C	0.9800
Cr2—Cg2	1.805	C31—C33	1.529 (4)
C1—C2	1.424 (4)	C31—C32	1.538 (4)
C1—C5	1.430 (4)	C31—C34	1.540 (4)
C1—C11	1.520 (4)	C32—H32A	0.9800
C2—C3	1.422 (4)	C32—H32B	0.9800
C2—H2	0.9500	C32—H32C	0.9800
C3—C4	1.420 (4)	C33—H33A	0.9800
C3—C31	1.525 (4)	C33—H33B	0.9800
C4—C5	1.429 (4)	C33—H33C	0.9800
C4—H4	0.9500	C34—H34A	0.9800
C5—H5	0.9500	C34—H34B	0.9800
C6—C7	1.420 (4)	C34—H34C	0.9800
C6—C10	1.425 (4)	C81—C83	1.524 (4)
C6—C61	1.526 (4)	C81—C84	1.525 (4)
C7—C8	1.416 (4)	C81—C82	1.541 (4)
C7—H7	0.9500	C82—H82A	0.9800
C8—C9	1.432 (4)	C82—H82B	0.9800
C8—C81	1.527 (4)	C82—H82C	0.9800
C9—C10	1.424 (4)	C83—H83A	0.9800
C9—H9	0.9500	C83—H83B	0.9800
C10—H10	0.9500	C83—H83C	0.9800
C11—C12	1.529 (4)	C84—H84A	0.9800
C11—C14	1.536 (4)	C84—H84B	0.9800
C11—C13	1.536 (4)	C84—H84C	0.9800
Cg1^{i}—Cr1—Cg1	173.3	C10—C6—C61	125.4 (3)
Cg2^{ii}—Cr2—Cg2	173.1	C7—C6—Cr2	71.66 (16)
C5^{i}—Cr1—C5	104.13 (16)	C10—C6—Cr2	67.29 (15)
C5^{i}—Cr1—C4^{i}	39.34 (10)	C61—C6—Cr2	130.32 (19)
C5—Cr1—C4^{i}	126.08 (11)	C8—C7—C6	110.3 (2)
C5^{i}—Cr1—C4	126.08 (11)	C8—C7—Cr2	69.33 (15)
C5—Cr1—C4	39.34 (10)	C6—C7—Cr2	71.16 (16)
C4^{i}—Cr1—C4	162.75 (15)	C8—C7—H7	124.8
C5^{i}—Cr1—C1^{i}	38.89 (10)	C6—C7—H7	124.8
C5—Cr1—C1^{i}	115.10 (11)	Cr2—C7—H7	126.3
C4^{i}—Cr1—C1^{i}	65.00 (11)	C7—C8—C9	106.2 (2)
C4—Cr1—C1^{i}	109.65 (11)	C7—C8—C81	127.4 (2)

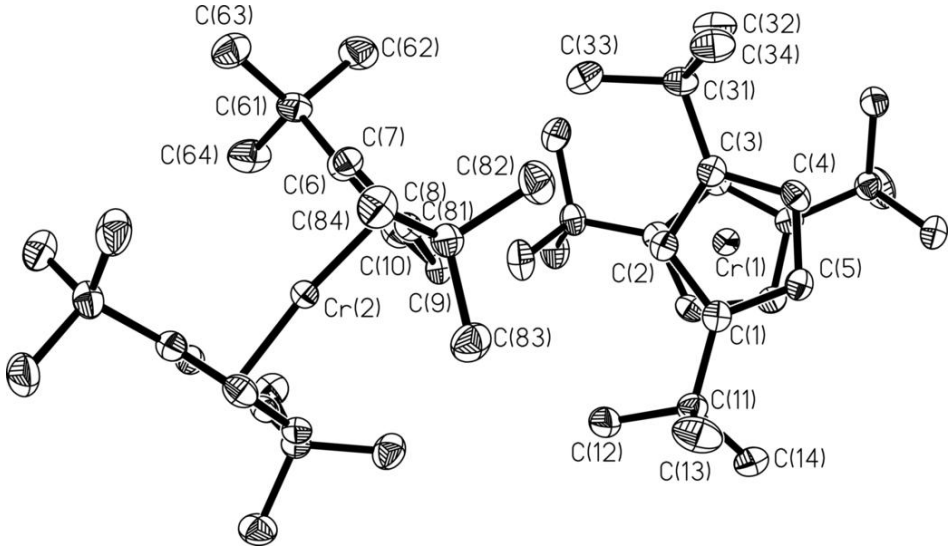
C5^{i}—Cr1—C1	115.09 (11)	C9—C8—C81	125.8 (3)
C5—Cr1—C1	38.89 (10)	C7—C8—Cr2	73.23 (16)
C4^{i}—Cr1—C1	109.65 (11)	C9—C8—Cr2	67.67 (15)
C4—Cr1—C1	65.00 (11)	C81—C8—Cr2	130.35 (19)
C1^{i}—Cr1—C1	146.51 (15)	C10—C9—C8	108.6 (3)
C5^{i}—Cr1—C2^{i}	63.43 (10)	C10—C9—Cr2	71.23 (15)
C5—Cr1—C2^{i}	149.79 (10)	C8—C9—Cr2	73.33 (15)
C4^{i}—Cr1—C2^{i}	62.92 (11)	C10—C9—H9	125.7
C4—Cr1—C2^{i}	123.85 (11)	C8—C9—H9	125.7
C1^{i}—Cr1—C2^{i}	37.70 (10)	Cr2—C9—H9	121.4
C1—Cr1—C2^{i}	170.62 (10)	C9—C10—C6	108.3 (3)
C5^{i}—Cr1—C2	149.79 (10)	C9—C10—Cr2	69.44 (15)
C5—Cr1—C2	63.43 (10)	C6—C10—Cr2	74.57 (16)
C4^{i}—Cr1—C2	123.85 (11)	C9—C10—H10	125.9
C4—Cr1—C2	62.92 (11)	C6—C10—H10	125.9
C1^{i}—Cr1—C2	170.62 (10)	Cr2—C10—H10	121.8
C1—Cr1—C2	37.70 (10)	C1—C11—C12	112.0 (2)
C2^{i}—Cr1—C2	140.35 (14)	C1—C11—C14	111.3 (2)
C5^{i}—Cr1—C3^{i}	64.46 (11)	C12—C11—C14	108.1 (2)
C5—Cr1—C3^{i}	163.88 (11)	C1—C11—C13	107.3 (2)
C4^{i}—Cr1—C3^{i}	37.93 (10)	C12—C11—C13	108.8 (2)
C4—Cr1—C3^{i}	156.62 (11)	C14—C11—C13	109.2 (3)
C1^{i}—Cr1—C3^{i}	63.98 (10)	C11—C12—H12A	109.5
C1—Cr1—C3^{i}	133.38 (10)	C11—C12—H12B	109.5
C2^{i}—Cr1—C3^{i}	37.24 (10)	H12A—C12—H12B	109.5
C2—Cr1—C3^{i}	120.26 (10)	C11—C12—H12C	109.5
C5^{i}—Cr1—C3	163.88 (11)	H12A—C12—H12C	109.5
C5—Cr1—C3	64.46 (11)	H12B—C12—H12C	109.5
C4^{i}—Cr1—C3	156.62 (11)	C11—C13—H13A	109.5
C4—Cr1—C3	37.93 (10)	C11—C13—H13B	109.5
C1^{i}—Cr1—C3	133.38 (10)	H13A—C13—H13B	109.5
C1—Cr1—C3	63.98 (10)	C11—C13—H13C	109.5
C2^{i}—Cr1—C3	120.26 (10)	H13A—C13—H13C	109.5
C2—Cr1—C3	37.24 (10)	H13B—C13—H13C	109.5
C3^{i}—Cr1—C3	128.98 (14)	C11—C14—H14A	109.5
C9^{ii}—Cr2—C9	103.90 (16)	C11—C14—H14B	109.5
C9^{ii}—Cr2—C10	125.26 (11)	H14A—C14—H14B	109.5
C9—Cr2—C10	39.32 (11)	C11—C14—H14C	109.5
C9^{ii}—Cr2—C10^{ii}	39.32 (11)	H14A—C14—H14C	109.5
C9—Cr2—C10^{ii}	125.26 (11)	H14B—C14—H14C	109.5
C10—Cr2—C10^{ii}	161.68 (16)	C63—C61—C6	110.8 (2)
C9^{ii}—Cr2—C8^{ii}	39.01 (10)	C63—C61—C64	109.4 (3)

C9—Cr2—C8^{ii}	115.49 (11)	C6—C61—C64	111.3 (2)
C10—Cr2—C8^{ii}	109.31 (11)	C63—C61—C62	109.1 (2)
C10^{ii}—Cr2—C8^{ii}	65.15 (11)	C6—C61—C62	107.5 (2)
C9^{ii}—Cr2—C8	115.49 (11)	C64—C61—C62	108.7 (3)
C9—Cr2—C8	39.01 (10)	C61—C62—H62A	109.5
C10—Cr2—C8	65.15 (11)	C61—C62—H62B	109.5
C10^{ii}—Cr2—C8	109.31 (11)	H62A—C62—H62B	109.5
C8^{ii}—Cr2—C8	147.33 (15)	C61—C62—H62C	109.5
C9^{ii}—Cr2—C6	163.24 (11)	H62A—C62—H62C	109.5
C9—Cr2—C6	64.40 (11)	H62B—C62—H62C	109.5
C10—Cr2—C6	38.14 (10)	C61—C63—H63A	109.5
C10^{ii}—Cr2—C6	157.26 (11)	C61—C63—H63B	109.5
C8^{ii}—Cr2—C6	132.93 (10)	H63A—C63—H63B	109.5
C8—Cr2—C6	63.81 (10)	C61—C63—H63C	109.5
C9^{ii}—Cr2—C6^{ii}	64.40 (11)	H63A—C63—H63C	109.5
C9—Cr2—C6^{ii}	163.24 (11)	H63B—C63—H63C	109.5
C10—Cr2—C6^{ii}	157.26 (11)	C61—C64—H64A	109.5
C10^{ii}—Cr2—C6^{ii}	38.14 (10)	C61—C64—H64B	109.5
C8^{ii}—Cr2—C6^{ii}	63.81 (10)	H64A—C64—H64B	109.5
C8—Cr2—C6^{ii}	132.93 (10)	C61—C64—H64C	109.5
C6—Cr2—C6^{ii}	129.54 (15)	H64A—C64—H64C	109.5
C9^{ii}—Cr2—C7	150.22 (11)	H64B—C64—H64C	109.5
C9—Cr2—C7	63.31 (11)	C3—C31—C33	111.6 (2)
C10—Cr2—C7	63.07 (11)	C3—C31—C32	111.1 (2)
C10^{ii}—Cr2—C7	124.13 (11)	C33—C31—C32	109.1 (2)
C8^{ii}—Cr2—C7	170.09 (10)	C3—C31—C34	108.0 (2)
C8—Cr2—C7	37.44 (10)	C33—C31—C34	108.5 (2)
C6—Cr2—C7	37.18 (10)	C32—C31—C34	108.5 (2)
C6^{ii}—Cr2—C7	120.48 (10)	C31—C32—H32A	109.5
C9^{ii}—Cr2—C7^{ii}	63.31 (11)	C31—C32—H32B	109.5
C9—Cr2—C7^{ii}	150.22 (11)	H32A—C32—H32B	109.5
C10—Cr2—C7^{ii}	124.13 (11)	C31—C32—H32C	109.5
C10^{ii}—Cr2—C7^{ii}	63.07 (11)	H32A—C32—H32C	109.5
C8^{ii}—Cr2—C7^{ii}	37.44 (10)	H32B—C32—H32C	109.5
C8—Cr2—C7^{ii}	170.09 (10)	C31—C33—H33A	109.5
C6—Cr2—C7^{ii}	120.48 (10)	C31—C33—H33B	109.5
C6^{ii}—Cr2—C7^{ii}	37.18 (10)	H33A—C33—H33B	109.5
C7—Cr2—C7^{ii}	140.28 (15)	C31—C33—H33C	109.5
C2—C1—C5	106.2 (2)	H33A—C33—H33C	109.5
C2—C1—C11	126.7 (2)	H33B—C33—H33C	109.5
C5—C1—C11	126.6 (3)	C31—C34—H34A	109.5
C2—C1—Cr1	72.89 (15)	C31—C34—H34B	109.5
C5—C1—Cr1	67.96 (15)	H34A—C34—H34B	109.5

C11—C1—Cr1	130.08 (19)	C31—C34—H34C	109.5
C3—C2—C1	110.3 (2)	H34A—C34—H34C	109.5
C3—C2—Cr1	71.48 (16)	H34B—C34—H34C	109.5
C1—C2—Cr1	69.41 (15)	C83—C81—C84	108.8 (2)
C3—C2—H2	124.8	C83—C81—C8	111.2 (2)
C1—C2—H2	124.8	C84—C81—C8	111.1 (2)
Cr1—C2—H2	125.9	C83—C81—C82	108.9 (2)
C4—C3—C2	106.4 (2)	C84—C81—C82	109.0 (2)
C4—C3—C31	126.3 (3)	C8—C81—C82	107.7 (2)
C2—C3—C31	127.1 (3)	C81—C82—H82A	109.5
C4—C3—Cr1	67.41 (15)	C81—C82—H82B	109.5
C2—C3—Cr1	71.28 (15)	H82A—C82—H82B	109.5
C31—C3—Cr1	130.19 (19)	C81—C82—H82C	109.5
C3—C4—C5	108.8 (3)	H82A—C82—H82C	109.5
C3—C4—Cr1	74.66 (16)	H82B—C82—H82C	109.5
C5—C4—Cr1	69.49 (15)	C81—C83—H83A	109.5
C3—C4—H4	125.6	C81—C83—H83B	109.5
C5—C4—H4	125.6	H83A—C83—H83B	109.5
Cr1—C4—H4	121.9	C81—C83—H83C	109.5
C4—C5—C1	108.3 (3)	H83A—C83—H83C	109.5
C4—C5—Cr1	71.16 (15)	H83B—C83—H83C	109.5
C1—C5—Cr1	73.16 (16)	C81—C84—H84A	109.5
C4—C5—H5	125.8	C81—C84—H84B	109.5
C1—C5—H5	125.8	H84A—C84—H84B	109.5
Cr1—C5—H5	121.6	C81—C84—H84C	109.5
C7—C6—C10	106.6 (3)	H84A—C84—H84C	109.5
C7—C6—C61	127.7 (3)	H84B—C84—H84C	109.5
C1—C2—C3—C4	0.2 (3)	C7—C6—C61—C63	−14.4 (4)
C1—C2—C3—C31	−174.6 (3)	C10—C6—C61—C63	172.3 (3)
C2—C3—C4—C5	−0.5 (3)	Cr2—C6—C61—C63	83.3 (3)
C31—C3—C4—C5	174.3 (2)	C7—C6—C61—C64	−136.4 (3)
C3—C4—C5—C1	0.6 (3)	C10—C6—C61—C64	50.3 (4)
C2—C1—C5—C4	−0.5 (3)	C7—C6—C61—C62	104.7 (3)
C6—C7—C8—C9	0.5 (3)	C10—C6—C61—C62	−68.7 (4)
C6—C7—C8—C81	172.1 (3)	C4—C3—C31—C33	171.3 (3)
C7—C8—C9—C10	−0.7 (3)	C2—C3—C31—C33	−14.9 (4)
C81—C8—C9—C10	−172.6 (2)	C4—C3—C31—C32	49.4 (4)
C8—C9—C10—C6	0.7 (3)	C2—C3—C31—C32	−136.8 (3)
C7—C6—C10—C9	−0.4 (3)	C4—C3—C31—C34	−69.5 (4)
C61—C6—C10—C9	174.1 (2)	C2—C3—C31—C34	104.3 (3)
C2—C1—C11—C12	36.7 (4)	C7—C8—C81—C83	150.6 (3)
C5—C1—C11—C12	−152.6 (3)	C9—C8—C81—C83	−39.3 (4)
C2—C1—C11—C14	157.9 (3)	C7—C8—C81—C84	29.2 (4)
C5—C1—C11—C14	−31.4 (4)	C9—C8—C81—C84	−160.7 (3)
C2—C1—C11—C13	−82.7 (3)	C7—C8—C81—C82	−90.1 (3)
C5—C1—C11—C13	88.0 (3)	C9—C8—C81—C82	80.0 (3)

Symmetry codes: (i) −*x*+1/2, −*y*+3/2, *z*; (ii) −*x*+1/2, −*y*+1/2, *z*.

Fig. 1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