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Racemic tricarbonyl[(4a,5,6,7,8,8a- η)-2-phenyl-3,4-dihydro-2H-1-benzopyran]-chromium(0)

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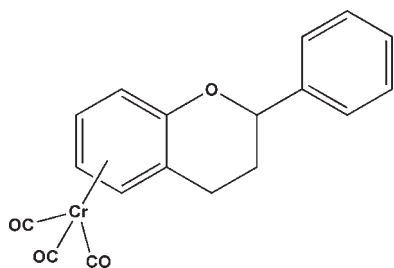
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.038; wR factor = 0.097; data-to-parameter ratio = 25.7.

The title compound, $[\text{Cr}(\text{C}_{15}\text{H}_{14}\text{O})(\text{CO})_3]$, displays a distorted envelope configuration of the dihydropyran ring. The dihedral angle between the phenyl and phenylene rings is $50.63(4)^\circ$. The Cr^0 atom is coordinated by three CO groups and the phenylene ring of the flavan ligand in an η^6 mode, with a common arene-to-metal distance

Related literature

For general background to chromium(0) complexes of the type $[\text{Cr}(\text{flav})(\text{CO})_3]$ (flav = flavan, flavone or isoflavone ligand), see: Muschalek *et al.* (2007). For related structures, see: van Tonder *et al.* (2009a,b). For the synthesis, see: Müller *et al.* (1999).



Experimental

Crystal data

$[\text{Cr}(\text{C}_{15}\text{H}_{14}\text{O})(\text{CO})_3]$
 $M_r = 346.29$
Monoclinic, $P2_1/c$
 $a = 12.0275(2)$ Å
 $b = 13.1454(2)$ Å
 $c = 10.4473(2)$ Å
 $\beta = 111.717(1)^\circ$

$V = 1534.55(5)$ Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 0.76$ mm⁻¹
 $T = 173$ K
 $0.46 \times 0.34 \times 0.11$ mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\min} = 0.766$, $T_{\max} = 0.938$

20468 measured reflections
5342 independent reflections
3728 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.050$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$
 $wR(F^2) = 0.097$
 $S = 0.95$
5342 reflections

208 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.67$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.32$ e Å⁻³

Table 1

Selected bond lengths (Å).

C5—Cr	2.1936 (18)	C10—Cr	2.2532 (17)
C6—Cr	2.2163 (19)	C11—Cr	1.8353 (19)
C7—Cr	2.2087 (19)	C12—Cr	1.8298 (19)
C8—Cr	2.2251 (17)	C13—Cr	1.8399 (17)
C9—Cr	2.2773 (17)		

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT-Plus (Bruker, 2007); data reduction: SAINT-Plus; program(s) used to solve structure: SIR97 (Altomare *et al.*, 1999); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg & Putz, 1999); software used to prepare material for publication: WinGX (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2329).

References

- Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
- Brandenburg, K. & Putz, H. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
- Bruker (2001). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2007). *APEX2* and *SAINTE-Plus*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
- Müller, T. J. J., Ansorge, M. & Polburn, K. (1999). *J. Organomet. Chem.* **578**, 252–259.
- Muschalek, B., Weidner, I. & Butenschön, H. (2007). *J. Organomet. Chem.* **692**, 2415–2424.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Tonder, J. H. van, Bezuidenhoudt, B. C. B. & Janse van Rensburg, J. M. (2009a). *Acta Cryst.* **E65**, m1343.
- Tonder, J. H. van, Bezuidenhoudt, B. C. B. & Janse van Rensburg, J. M. (2009b). *Acta Cryst.* **E65**, m1346.

supporting information

Acta Cryst. (2010). E66, m1086 [https://doi.org/10.1107/S1600536810031028]

Racemic tricarbonyl[(4a,5,6,7,8,8a- η)-2-phenyl-3,4-dihydro-2H-1-benzopyran]-chromium(0)

Johannes H. van Tonder, Barend C. B. Bezuidenhoudt and J. Marthinus Janse van Rensburg

S1. Comment

The title compound forms part of a series of chromium(0) complexes of the type [Cr(flav)(CO)₃] (flav = flavan, flavone or isoflavone ligand) (van Tonder *et al.*, 2009a,b). Our interest in this type of chromium(0) complexes is partly due to their importance in organic synthesis, as noted earlier (Muschalek *et al.*, 2007).

As illustrated in Fig. 1, the Cr(CO)₃ group coordinates to the phenylene ring of the flavanoid backbone (Table 1). The distance between the Cr⁰ atom and the centroid of the A- η^6 -coordinated arene ring is 1.731 (1) Å (r.m.s of fitted atoms C5–C10 = 0.0186 Å). Molecular distortion is displayed by the twisted flavan backbone. Atoms C4 and O5 is essentially in the plane of the coordinated arene ring (r.m.s of atoms C4–C10 and O5 = 0.0202 Å), while atoms C2 and C3 are respectively displaced by -0.244 (2) and 0.478 (2) Å from the plane formed by atoms C4–C10 and O5. This distortion is a result of the expected envelope configuration in the dihydropyran ring. In turn the phenyl ring is twisted away from the plane of atoms C4–C10 and O5, with a dihedral angle of 50.88 (4)°. The crystal packing displays an intermolecular C—H \cdots π soft contact [H \cdots centroid distance = 2.92 Å] between the phenyl ring of one molecule and the arene ring of a neighbouring molecule (Fig. 2). The crystal packing is also stabilized by a C—H \cdots O soft contact between atoms H8 and O5, with a distance of 2.57 Å and a C8—H8 \cdots O5 angle of 140°.

S2. Experimental

Flavan was synthesized via H₂SO₄ catalyzed hydrogenation (5 bar) over 10% Pd/C from flavan-4-one [flavan-4-one (2.00 g, 8.9 mmol), 10 % Pd/C (0.10 g), 3 M H₂SO₄ (1 ml), EtOH (50 ml)]. Purification by means of flash column-chromatography yielded flavan (0.94 g, 49.9%) as a colourless oil. R_f 0.77 (H:A, 8:2).

Preparation of the title compound was based on a method described by Müller *et al.* (1999). A solution of flavan (0.51 g, 2.4 mmol) and Cr(CO)₆ (0.53 g, 2.4 mmol) in Bu₂O:THF (9:1, 10 ml per 100 mg) was degassed with argon, using standard Schlenk techniques, and refluxed (48 h) under an oxygen free atmosphere. The reaction mixture was cooled to room temperature and the solvent evaporated in vacuo. Purification through flash column-chromatography yielded tricarbonyl(A- η^6 flavan)chromium(0) (0.08 g, 9.2%) as a yellow solid. Recrystallization from diethyl ether yielded yellow cuboidal crystals. R_f 0.23 (hexane:acetone, 8:2); Mp 170.4°C.

S3. Refinement

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 (aromatic), 0.98 (CH) and 0.97 (CH₂) Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

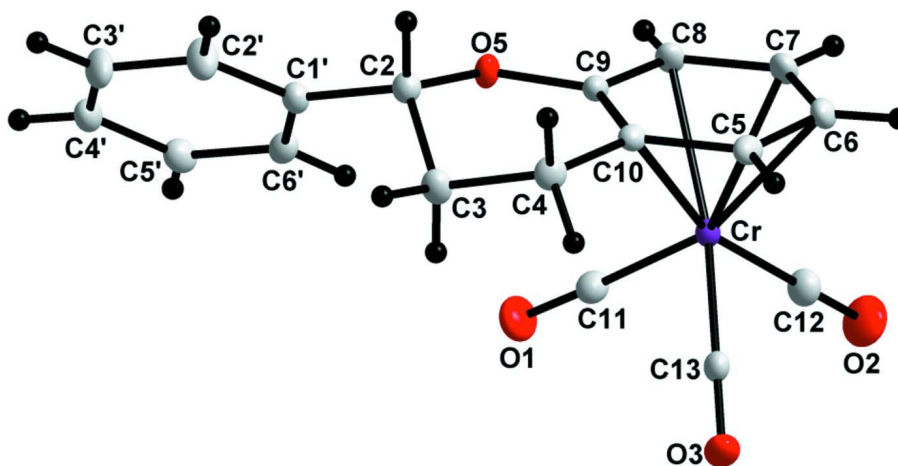


Figure 1
Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

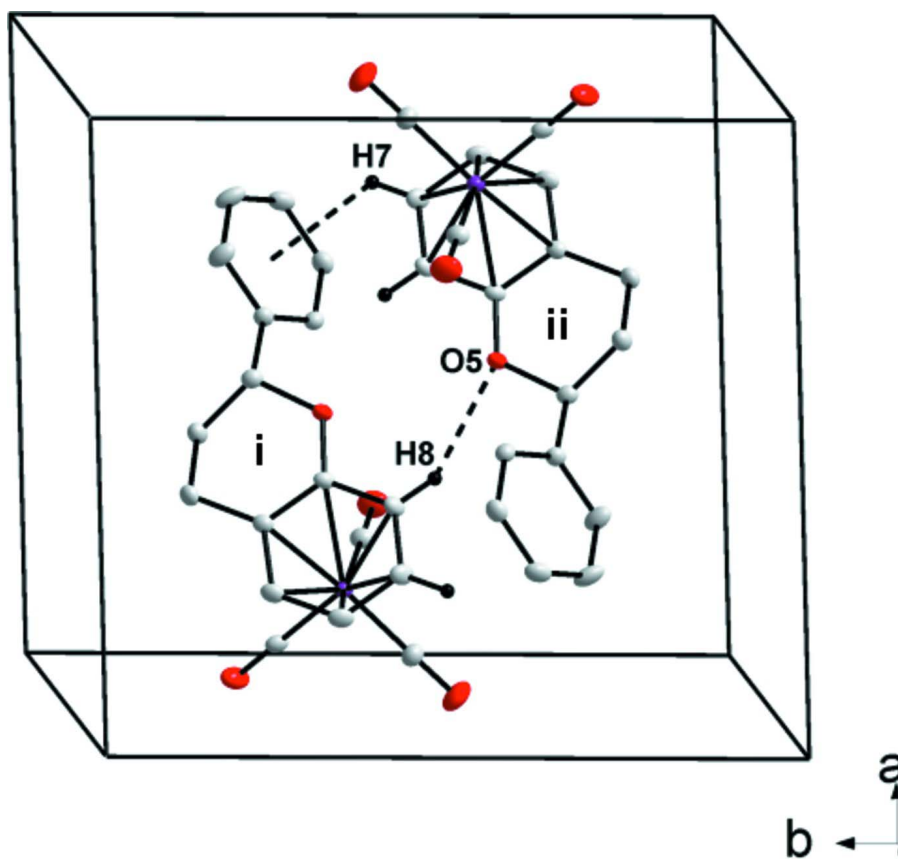


Figure 2
A view of the crystal packing in the unit cell. [Symmetry codes: (i) $1-x, 1/2+y, 1/2-z$; (ii) $x, 1/2-y, 1/2+z$.]

tricarbonyl[(4a,5,6,7,8,8a- η)-2-phenyl-3,4-dihydro-2H-1-benzopyran]chromium(0)*Crystal data*[Cr(C₁₅H₁₄O)(CO)₃] $M_r = 346.29$ Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

 $a = 12.0275 (2) \text{ \AA}$ $b = 13.1454 (2) \text{ \AA}$ $c = 10.4473 (2) \text{ \AA}$ $\beta = 111.717 (1)^\circ$ $V = 1534.55 (5) \text{ \AA}^3$ $Z = 4$ $F(000) = 712$ $D_x = 1.499 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71069 \text{ \AA}$

Cell parameters from 4557 reflections

 $\theta = 2.4\text{--}30.0^\circ$ $\mu = 0.76 \text{ mm}^{-1}$ $T = 173 \text{ K}$

Plate, yellow

 $0.46 \times 0.34 \times 0.11 \text{ mm}$ *Data collection*

Bruker APEXII CCD

diffractometer

Graphite monochromator

 φ and ω scans

Absorption correction: multi-scan

(SADABS; Bruker, 2001)

 $T_{\min} = 0.766$, $T_{\max} = 0.938$

20468 measured reflections

5342 independent reflections

3728 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.050$ $\theta_{\max} = 32.1^\circ$, $\theta_{\min} = 1.8^\circ$ $h = -17 \rightarrow 14$ $k = -19 \rightarrow 19$ $l = -14 \rightarrow 15$ *Refinement*Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.038$ $wR(F^2) = 0.097$ $S = 0.95$

5342 reflections

208 parameters

0 restraints

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

 $w = 1/[\sigma^2(F_o^2) + (0.0469P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} = 0.001$ $\Delta\rho_{\max} = 0.67 \text{ e \AA}^{-3}$ $\Delta\rho_{\min} = -0.32 \text{ e \AA}^{-3}$ *Special details***Experimental.** The intensity data was collected on a Bruker APEXII CCD diffractometer using a frame width of 0.5° covering up to $\theta = 32.06^\circ$ with 99.8% completeness accomplished.Spectroscopic data for the flavan ligand: $^1\text{H NMR}$ (CDCl_3 , 600 MHz) δ p.p.m. 7.46 – 7.30 (5H, m, Ar—H), 7.21 – 7.10 (2H, m, Ar—H), 6.94 – 6.86 (2H, m, Ar—H), 5.08 (1H, dd, $J = 2.45$, 9.98 Hz), 3.02 (1H, ddd, $J = 6.03$, 11.02, 16.46 Hz), 2.81 (1H, ddd, $J = 3.58$, 4.71, 16.46 Hz), 2.27 – 2.04 (2H, m); $^{13}\text{C NMR}$ (600 MHz, CDCl_3) δ p.p.m. 25.18, 30.06, 77.82, 117.04, 120.43, 121.93, 126.10, 127.45, 127.91, 128.61, 129.63, 141.87, 155.25.Spectroscopic data for the title compound, tricarbonyl(A- η^6 flavan)chromium(0): Note: A, B and C-ring labelling refers to the benzene, phenyl and dihydropyran rings respectively. $^1\text{H NMR}$ (600 MHz, CDCl_3) δ p.p.m. 7.46 (2H, d, $J = 7.30$ Hz), 7.40 (2H, dd, $J = 7.24$, 7.30 Hz), 7.37 – 7.35 (1H, m), 5.56 (1H, d, $J = 6.03$ Hz), 5.48 (1H, dd, $J = 6.02$, 6.69 Hz), 5.20 (1H, d, $J = 6.69$ Hz), 4.90 – 4.88 (2H, m), 3.00 (1H, ddd, $J = 5.27$, 12.42, 15.95 Hz), 2.64 (1H, dd, $J = 4.14$, 15.95 Hz), 2.31 (1H, ddd, $J = 4.14$, 12.42, 13.93 Hz), 2.17 (1H, dd, $J = 5.27$, 13.93 Hz); $^{13}\text{C NMR}$ (600 MHz, CDCl_3) δ p.p.m. 25.94 (C-4), 29.67 (C-3), 80.00 (C-2/6/8), 80.29 (C-2/6/8), 85.87 (C-2/6/8), 94.50 (C-5/7), 95.60 (C-5/7), 126.49 (C-2' and C-6'), 128.80, 128.89, 139.71, 234.06 (–Cr(CO)₃);MS m/z 346 (M^+ , 39.0), 290 (2.7), 263 (22.1), 222 (56.9), 193 (12.0), 167 (100.0), 158 (99.8), 149 (68.9), 129 (1.9), 127 (13.0), 121 (27.0), 106 (31.3), 104 (4.8), 103 (7.8).

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1'	0.42382 (14)	0.18308 (12)	0.19968 (17)	0.0245 (3)
C2	0.50936 (14)	0.20966 (13)	0.12917 (17)	0.0263 (3)
H2	0.4643	0.2420	0.0405	0.032*
C2'	0.32347 (17)	0.24327 (15)	0.1760 (2)	0.0372 (4)
H2'	0.3095	0.2986	0.1167	0.045*
C3	0.60863 (15)	0.27990 (13)	0.21249 (18)	0.0293 (4)
H3A	0.6526	0.2491	0.3013	0.035*
H3B	0.5746	0.3433	0.2285	0.035*
C3'	0.24388 (17)	0.22168 (16)	0.2401 (2)	0.0405 (5)
H3'	0.1772	0.2629	0.2240	0.049*
C4	0.69396 (15)	0.30169 (12)	0.13848 (18)	0.0269 (3)
H4A	0.6552	0.3457	0.0600	0.032*
H4B	0.7645	0.3364	0.2005	0.032*
C4'	0.26295 (15)	0.13974 (15)	0.32735 (18)	0.0327 (4)
H4'	0.2084	0.1245	0.3686	0.039*
C5'	0.36356 (16)	0.08021 (13)	0.35341 (18)	0.0295 (4)
H5'	0.3773	0.0254	0.4135	0.035*
C5	0.83325 (14)	0.19620 (13)	0.05541 (16)	0.0261 (3)
H5	0.8817	0.2531	0.0654	0.031*
C6'	0.44412 (14)	0.10155 (12)	0.29068 (18)	0.0260 (3)
H6'	0.5119	0.0614	0.3094	0.031*
C6	0.86366 (15)	0.10536 (13)	0.00632 (17)	0.0290 (4)
H6	0.9293	0.1028	-0.0204	0.035*
C7	0.79393 (15)	0.01836 (14)	-0.00212 (18)	0.0309 (4)
H7	0.8147	-0.0427	-0.0322	0.037*
C8	0.69312 (14)	0.02274 (13)	0.03445 (17)	0.0278 (4)
H8	0.6488	-0.0357	0.0319	0.033*
C9	0.65942 (13)	0.11637 (12)	0.07510 (16)	0.0223 (3)
C10	0.72998 (13)	0.20345 (12)	0.09035 (15)	0.0219 (3)
C11	0.79274 (15)	0.03598 (13)	0.34020 (18)	0.0297 (4)
C12	0.96333 (16)	-0.02379 (14)	0.26452 (19)	0.0334 (4)
C13	0.95879 (14)	0.16059 (13)	0.34028 (17)	0.0267 (3)
O1	0.75227 (13)	0.00961 (11)	0.41970 (15)	0.0468 (4)
O2	1.03289 (14)	-0.08866 (11)	0.29813 (18)	0.0576 (4)
O3	1.02610 (11)	0.21213 (11)	0.42255 (14)	0.0422 (3)
O5	0.55780 (9)	0.11377 (8)	0.10382 (12)	0.0260 (2)
Cr	0.85184 (2)	0.078021 (19)	0.21024 (3)	0.02026 (7)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1'	0.0243 (7)	0.0262 (8)	0.0257 (8)	-0.0011 (6)	0.0126 (6)	-0.0017 (6)
C2	0.0242 (8)	0.0296 (8)	0.0261 (8)	0.0011 (6)	0.0106 (6)	0.0006 (7)
C2'	0.0396 (10)	0.0401 (10)	0.0380 (10)	0.0150 (8)	0.0215 (8)	0.0135 (8)
C3	0.0306 (9)	0.0270 (8)	0.0338 (9)	-0.0040 (6)	0.0160 (7)	-0.0058 (7)

C3'	0.0318 (9)	0.0562 (12)	0.0377 (10)	0.0187 (9)	0.0179 (8)	0.0066 (9)
C4	0.0286 (8)	0.0225 (7)	0.0312 (9)	-0.0040 (6)	0.0131 (7)	0.0017 (7)
C4'	0.0264 (8)	0.0472 (11)	0.0288 (9)	-0.0049 (7)	0.0152 (7)	-0.0042 (8)
C5'	0.0336 (9)	0.0287 (8)	0.0288 (9)	-0.0049 (7)	0.0147 (7)	0.0016 (7)
C5	0.0237 (8)	0.0346 (9)	0.0218 (8)	-0.0047 (6)	0.0105 (6)	0.0040 (7)
C6'	0.0226 (8)	0.0257 (8)	0.0296 (9)	0.0014 (6)	0.0094 (6)	-0.0017 (7)
C6	0.0251 (8)	0.0436 (10)	0.0229 (8)	-0.0020 (7)	0.0140 (6)	-0.0025 (7)
C7	0.0283 (8)	0.0389 (10)	0.0277 (9)	-0.0027 (7)	0.0131 (7)	-0.0133 (8)
C8	0.0247 (8)	0.0316 (9)	0.0283 (8)	-0.0079 (6)	0.0112 (7)	-0.0119 (7)
C9	0.0182 (7)	0.0304 (8)	0.0189 (7)	-0.0032 (6)	0.0075 (6)	-0.0037 (6)
C10	0.0212 (7)	0.0267 (8)	0.0181 (7)	-0.0016 (6)	0.0076 (6)	0.0020 (6)
C11	0.0268 (8)	0.0330 (9)	0.0288 (9)	0.0007 (7)	0.0096 (7)	0.0045 (7)
C12	0.0334 (9)	0.0314 (9)	0.0372 (10)	0.0039 (7)	0.0150 (8)	-0.0010 (8)
C13	0.0208 (7)	0.0347 (9)	0.0263 (8)	0.0028 (6)	0.0106 (6)	-0.0032 (7)
O1	0.0496 (9)	0.0583 (9)	0.0418 (8)	0.0003 (7)	0.0278 (7)	0.0146 (7)
O2	0.0532 (10)	0.0460 (9)	0.0714 (12)	0.0253 (7)	0.0206 (9)	0.0070 (8)
O3	0.0290 (7)	0.0562 (8)	0.0387 (7)	-0.0062 (6)	0.0091 (6)	-0.0196 (7)
O5	0.0200 (5)	0.0275 (6)	0.0347 (6)	-0.0051 (4)	0.0149 (5)	-0.0083 (5)
Cr	0.01890 (12)	0.02262 (13)	0.02079 (13)	-0.00077 (9)	0.00912 (9)	-0.00132 (10)

Geometric parameters (Å, °)

C1'—C2'	1.387 (2)	C5—H5	0.9300
C1'—C6'	1.393 (2)	C6'—H6'	0.9300
C1'—C2	1.511 (2)	C6—C7	1.401 (2)
C2—O5	1.4535 (19)	C6—H6	0.9300
C2—C3	1.506 (2)	C7—C8	1.401 (2)
C2—H2	0.9800	C7—H7	0.9300
C2'—C3'	1.385 (3)	C8—C9	1.410 (2)
C2'—H2'	0.9300	C8—H8	0.9300
C3—C4	1.523 (2)	C9—O5	1.3627 (18)
C3—H3A	0.9700	C9—C10	1.399 (2)
C3—H3B	0.9700	C11—O1	1.160 (2)
C3'—C4'	1.374 (3)	C12—O2	1.155 (2)
C3'—H3'	0.9300	C13—O3	1.157 (2)
C4—C10	1.506 (2)	C5—Cr	2.1936 (18)
C4—H4A	0.9700	C6—Cr	2.2163 (19)
C4—H4B	0.9700	C7—Cr	2.2087 (19)
C4'—C5'	1.381 (2)	C8—Cr	2.2251 (17)
C4'—H4'	0.9300	C9—Cr	2.2773 (17)
C5'—C6'	1.384 (2)	C10—Cr	2.2532 (17)
C5'—H5'	0.9300	C11—Cr	1.8353 (19)
C5—C6	1.401 (2)	C12—Cr	1.8298 (19)
C5—C10	1.421 (2)	C13—Cr	1.8399 (17)
C2'—C1'—C6'	118.79 (15)	C9—C8—Cr	73.78 (9)
C2'—C1'—C2	119.07 (15)	C7—C8—H8	120.2
C6'—C1'—C2	122.11 (14)	C9—C8—H8	120.2

O5—C2—C3	110.59 (13)	Cr—C8—H8	127.0
O5—C2—C1'	106.22 (13)	O5—C9—C10	123.47 (14)
C3—C2—C1'	113.41 (14)	O5—C9—C8	115.20 (14)
O5—C2—H2	108.8	C10—C9—C8	121.26 (14)
C3—C2—H2	108.8	O5—C9—Cr	130.29 (11)
C1'—C2—H2	108.8	C10—C9—Cr	71.08 (9)
C3'—C2'—C1'	120.57 (17)	C8—C9—Cr	69.75 (9)
C3'—C2'—H2'	119.7	C9—C10—C5	117.84 (15)
C1'—C2'—H2'	119.7	C9—C10—C4	120.15 (13)
C2—C3—C4	111.16 (14)	C5—C10—C4	121.99 (14)
C2—C3—H3A	109.4	C9—C10—Cr	72.96 (9)
C4—C3—H3A	109.4	C5—C10—Cr	69.09 (9)
C2—C3—H3B	109.4	C4—C10—Cr	130.54 (11)
C4—C3—H3B	109.4	O1—C11—Cr	178.15 (15)
H3A—C3—H3B	108.0	O2—C12—Cr	179.38 (19)
C4'—C3'—C2'	120.36 (17)	O3—C13—Cr	179.64 (17)
C4'—C3'—H3'	119.8	C9—O5—C2	118.10 (12)
C2'—C3'—H3'	119.8	C12—Cr—C11	89.46 (8)
C10—C4—C3	109.83 (13)	C12—Cr—C13	88.32 (8)
C10—C4—H4A	109.7	C11—Cr—C13	89.30 (8)
C3—C4—H4A	109.7	C12—Cr—C5	127.56 (7)
C10—C4—H4B	109.7	C11—Cr—C5	142.85 (7)
C3—C4—H4B	109.7	C13—Cr—C5	88.82 (8)
H4A—C4—H4B	108.2	C12—Cr—C7	88.52 (8)
C3'—C4'—C5'	119.60 (16)	C11—Cr—C7	124.86 (8)
C3'—C4'—H4'	120.2	C13—Cr—C7	145.65 (7)
C5'—C4'—H4'	120.2	C5—Cr—C7	66.58 (7)
C4'—C5'—C6'	120.51 (16)	C12—Cr—C6	96.67 (8)
C4'—C5'—H5'	119.7	C11—Cr—C6	160.06 (7)
C6'—C5'—H5'	119.7	C13—Cr—C6	109.76 (7)
C6—C5—C10	121.51 (15)	C5—Cr—C6	37.03 (6)
C6—C5—Cr	72.37 (10)	C7—Cr—C6	36.93 (7)
C10—C5—Cr	73.65 (9)	C12—Cr—C8	108.88 (8)
C6—C5—H5	119.2	C11—Cr—C8	93.63 (8)
C10—C5—H5	119.2	C13—Cr—C8	162.56 (7)
Cr—C5—H5	126.7	C5—Cr—C8	78.49 (7)
C5'—C6'—C1'	120.15 (15)	C7—Cr—C8	36.83 (6)
C5'—C6'—H6'	119.9	C6—Cr—C8	66.43 (7)
C1'—C6'—H6'	119.9	C12—Cr—C10	163.51 (7)
C5—C6—C7	119.17 (15)	C11—Cr—C10	106.33 (7)
C5—C6—Cr	70.60 (9)	C13—Cr—C10	96.43 (7)
C7—C6—Cr	71.24 (9)	C5—Cr—C10	37.25 (6)
C5—C6—H6	120.4	C7—Cr—C10	78.64 (7)
C7—C6—H6	120.4	C6—Cr—C10	66.85 (6)
Cr—C6—H6	130.2	C8—Cr—C10	66.24 (6)
C8—C7—C6	120.50 (16)	C12—Cr—C9	144.51 (7)
C8—C7—Cr	72.22 (10)	C11—Cr—C9	86.69 (7)
C6—C7—Cr	71.83 (10)	C13—Cr—C9	126.85 (7)

C8—C7—H7	119.8	C5—Cr—C9	65.36 (6)
C6—C7—H7	119.8	C7—Cr—C9	65.51 (6)
Cr—C7—H7	128.5	C6—Cr—C9	77.30 (6)
C7—C8—C9	119.50 (15)	C8—Cr—C9	36.47 (6)
C7—C8—Cr	70.95 (10)	C10—Cr—C9	35.96 (5)
