Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

cis-Bis(acetylacetonato)diaquachromium(III) perchlorate monohydrate

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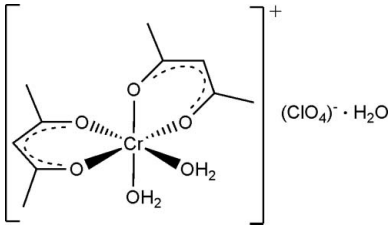
Received 17 July 2007; accepted 6 August 2007

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.005 Å; R factor = 0.048; wR factor = 0.158; data-to-parameter ratio = 17.6.

The Cr^{3+} center of the cation present in the title compound, $[Cr(C_5H_7O_2)_2(H_2O)_2]ClO_4\cdot H_2O$, assumes a pseudo-octahedral geometry. The uncoordinated water molecule and the perchlorate anion are involved in moderately strong O—H···O hydrogen-bonding interactions with the cation, resulting in a three-dimensional network.

Related literature

For synthesis, see: Ogino *et al.* (1988). Structural features observed for the cation in (I) are comparable to those reported for the cation in the corresponding tetrafluoridoborate salt (Nakano *et al.*, 2003). For related literature, see: Lemmer *et al.* (2002); Marinescu *et al.* (2002);



Experimental

Crystal data

$[Cr(C_5H_7O_2)_2(H_2O)_2]ClO_4\cdot H_2O$
M_r = 403.71
Monoclinic, $P2_1/n$
a = 9.9811 (3) Å
b = 14.8470 (5) Å
c = 12.0093 (4) Å
β = 96.036 (2)°
V = 1769.78 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.85 mm^{-1}
T = 296 (2) K
0.38 × 0.24 × 0.12 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004*a*)
T_{min} = 0.776, T_{max} = 0.894
38774 measured reflections
4051 independent reflections
2771 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.158
S = 1.11
4051 reflections
230 parameters
10 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cr1—O2	1.9306 (19)	Cr1—O1	1.947 (2)
Cr1—O3	1.9327 (19)	Cr1—O1*W*	1.991 (2)
Cr1—O4	1.9396 (19)	Cr1—O2*W*	2.009 (2)
O2—Cr1—O3	176.62 (8)	O4—Cr1—O1*W*	91.17 (9)
O2—Cr1—O4	90.34 (8)	O1—Cr1—O1*W*	179.15 (9)
O3—Cr1—O4	91.94 (8)	O2—Cr1—O2*W*	91.26 (9)
O2—Cr1—O1	92.32 (9)	O3—Cr1—O2*W*	86.51 (9)
O3—Cr1—O1	90.21 (9)	O4—Cr1—O2*W*	178.13 (8)
O4—Cr1—O1	89.28 (8)	O1—Cr1—O2*W*	89.69 (10)
O2—Cr1—O1*W*	86.96 (9)	O1*W*—Cr1—O2*W*	89.88 (10)
O3—Cr1—O1*W*	90.49 (9)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O4^{i}	0.833 (10)	1.96 (2)	2.791 (3)	174 (3)
O1*W*—H1*WB*···O3*W*	0.829 (10)	1.79 (1)	2.616 (3)	171 (3)
O2*W*—H2*WA*···O1^{ii}	0.830 (10)	1.96 (2)	2.778 (3)	169 (3)
O2*W*—H2*WB*···O7	0.839 (10)	1.84 (1)	2.675 (4)	173 (4)
O3*W*—H3*WA*···O8^{iii}	0.84 (4)	1.96 (2)	2.770 (5)	161 (6)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x, -y+1, -z+1$; (iii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2004*b*); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the College of Arts and Sciences, University of Wyoming, for financial support (Basic Research Grant).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2419).

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 doi:10.1107/S1600536807038688

supplementary materials

Acta Cryst. (2007). E**63**, m2307 [**doi:10.1107/S1600536807038688**]

cis-Bis(acetylacetonato)diaquachromium(III) perchlorate monohydrate

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Comment

Our interest in the title compound, (I), stems from its usefulness as a starting material for the synthesis of mixed ligand bis(acetylacetonato)Cr(III)-amino acidato complexes. We have obtained crystals of (I) as the major product together with the *trans* isomer from a modified literature procedure (Ogino *et al.*, 1988).

In compound (I), two acetylacetonato ligands and two water molecules bind the Cr^{3+} center conferring pseudo-octahedral geometry to the metal ion (Fig. 1). The ions and the solvated water molecules are linked through hydrogen bonding. The hydrogen bonding interaction between the ions gives rise to a three-dimensional network as shown in Fig. 2.

Specifically, one of the coordinated water molecules (O1W) is hydrogen bonded to the solvated water molecule (O3W), whereas the other (O2W) is hydrogen bonded to a perchlorate O atom (O7). Each of the two water molecules is hydrogen bonded to a coordinated acetylacetonato anion through one of the O atoms of the latter ligand. In addition, the solvated water molecule (O3W) is also involved in a moderately strong hydrogen bonding with one of the perchlorate O atoms (O8).

Unlike in the structure of the corresponding tetrafluroborate salt (Nakano *et al.*, 2003), the anion in (I) is ordered, possibly a consequence of the hydrogen bonds. The Cr—O_{acac} bonds are only slightly shorter (*ca* 0.06 Å) than the two Cr—O_{aqua} bonds indicating strong bonds with the water molecules as observed in the *trans*-bis(malonato)(diaqua)chromium(III) (Lemmer *et al.*, 2002) and *cis*-bis(oxalato)diaquachromium(III) cations (Marinescu *et al.*, 2002).

Experimental

Compound (I) was obtained by the ligand exchange reaction of [$Cr(acac)_3$] with water in the presene of perchloric acid by a modified literature procedure (Ogino *et al.*, 1988), as follows: To a suspension of [$Cr(acac)_3$] (6.981 g, 20 mmol) in water (200 ml) were added a solution of $HClO_4$ (3 ml, 70% *w*/*v*) in water (50 ml) and ethanol (95%, 50 ml). The mixture was allowed to reflux for 5 d. The reaction mixture was treated following the literature method, rotary evaporated to *ca* 15 ml and allowed to stand at room temperature overnight. The *cis* and *trans* isomers of the complex crystallized as large purple and brown-purple rectangular prisms, respectively. A purple crystal of suitable size was chosen for the X-ray diffraction studies.

Refinement

The water H atoms were located and refined, with the O—H and H···H distances restrained to 0.84 (1) and 1.37 (2) Å, respectively, and with $U_{iso}(H) = 1.5U_{eq}(O)$. Other H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.96 Å and $U_{iso}(H) = 1.2–1.5U_{eq}(C)$.

Figures

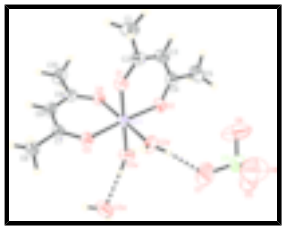

Fig. 1. The asymmetric unit of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres with arbitrary radii. Hydrogen bonds are represented by dashed lines.

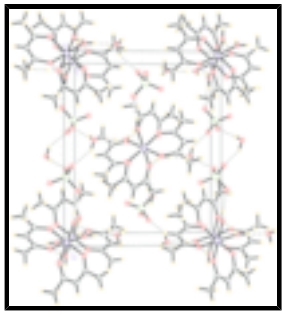

Fig. 2. The crystal packing of (I), viewed down the *a* axis.

cis-Bis(acetylacetonato)diaquachromium(III) perchlorate monohydrate

Crystal data

$[Cr(C_5H_7O_2)_2(H_2O)_2]ClO_4·H_2O$	F_{000} = 836
M_r = 403.71	D_x = 1.515 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 8910 reflections
a = 9.9811 (3) Å	θ = 2.2–24.4º
b = 14.8470 (5) Å	μ = 0.85 mm^{-1}
c = 12.0093 (4) Å	T = 296 (2) K
β = 96.036 (2)º	Rectangular prism, purple
V = 1769.78 (10) Å^3	0.38 × 0.24 × 0.12 mm
Z = 4	

Data collection

Bruker APEXII CCD area-detector diffractometer	4051 independent reflections
Radiation source: fine-focus sealed tube	2771 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.047
T = 296(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004a)	h = −12→12
T_{min} = 0.776, T_{max} = 0.894	k = −19→19
38774 measured reflections	l = −15→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.048$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.158$	$w = 1/[\sigma^2(F_o^2) + (0.0777P)^2 + 0.8712P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{max} = 0.013$
4051 reflections	$\Delta\rho_{max} = 0.64$ e Å^{-3}
230 parameters	$\Delta\rho_{min} = -0.48$ e Å^{-3}
10 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.24915 (4)	0.50161 (3)	0.49777 (3)	0.03861 (17)
O1	0.11295 (17)	0.46012 (14)	0.38113 (17)	0.0464 (5)
O1W	0.38847 (19)	0.54583 (18)	0.61600 (18)	0.0569 (6)

H1WA	0.4639 (19)	0.560 (3)	0.598 (3)	0.085*
H1WB	0.387 (3)	0.547 (3)	0.6849 (10)	0.085*
O2	0.32828 (19)	0.58155 (14)	0.39606 (17)	0.0495 (5)
O2W	0.1230 (2)	0.59873 (14)	0.5386 (2)	0.0586 (6)
H2WA	0.048 (2)	0.587 (2)	0.558 (3)	0.088*
H2WB	0.137 (3)	0.6545 (8)	0.541 (4)	0.088*
O3	0.17123 (19)	0.42715 (13)	0.60618 (16)	0.0461 (5)
O4	0.36654 (18)	0.40495 (13)	0.45914 (16)	0.0431 (4)
C1	0.0035 (4)	0.4301 (3)	0.2014 (3)	0.0719 (10)
H1A	0.0191	0.3663	0.2049	0.108*
H1B	0.0050	0.4505	0.1257	0.108*
H1C	−0.0829	0.4432	0.2261	0.108*
C2	0.1115 (3)	0.4776 (2)	0.2757 (3)	0.0509 (7)
C3	0.1994 (3)	0.5354 (2)	0.2309 (3)	0.0595 (8)
H3	0.1903	0.5414	0.1534	0.071*
C4	0.3003 (3)	0.5857 (2)	0.2903 (3)	0.0510 (7)
C5	0.3840 (4)	0.6505 (3)	0.2314 (3)	0.0771 (11)
H5A	0.3634	0.7110	0.2521	0.116*
H5B	0.3643	0.6433	0.1519	0.116*
H5C	0.4777	0.6386	0.2525	0.116*
C6	0.1033 (4)	0.3005 (2)	0.7020 (3)	0.0628 (9)
H6A	0.1092	0.3371	0.7682	0.094*
H6B	0.1378	0.2415	0.7208	0.094*
H6C	0.0110	0.2960	0.6710	0.094*
C7	0.1845 (3)	0.3426 (2)	0.6179 (2)	0.0441 (6)
C8	0.2686 (3)	0.2903 (2)	0.5606 (3)	0.0556 (8)
H8	0.2665	0.2285	0.5726	0.067*
C9	0.3560 (3)	0.3215 (2)	0.4869 (2)	0.0473 (7)
C10	0.4473 (4)	0.2596 (2)	0.4342 (4)	0.0744 (11)
H10A	0.4384	0.2694	0.3548	0.112*
H10B	0.4239	0.1984	0.4493	0.112*
H10C	0.5387	0.2708	0.4644	0.112*
Cl1	0.18174 (9)	0.84694 (6)	0.48642 (9)	0.0702 (3)
O5	0.2817 (4)	0.9075 (2)	0.5349 (3)	0.1088 (11)
O6	0.2096 (5)	0.8157 (3)	0.3860 (4)	0.166 (2)
O7	0.1774 (5)	0.7744 (2)	0.5643 (4)	0.1472 (16)
O8	0.0575 (4)	0.8874 (4)	0.4839 (4)	0.177 (2)
O3W	0.3564 (3)	0.5459 (2)	0.8294 (2)	0.0920 (9)
H3WB	0.348 (5)	0.4912 (10)	0.847 (2)	0.138*
H3WA	0.428 (3)	0.565 (3)	0.864 (4)	0.138*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.0244 (2)	0.0459 (3)	0.0472 (3)	−0.00116 (17)	0.01153 (18)	0.00286 (19)
O1	0.0274 (9)	0.0551 (12)	0.0573 (12)	−0.0027 (8)	0.0070 (8)	−0.0001 (9)
O1W	0.0329 (10)	0.0875 (16)	0.0521 (12)	−0.0158 (11)	0.0127 (9)	−0.0069 (12)
O2	0.0368 (10)	0.0561 (12)	0.0571 (13)	−0.0065 (9)	0.0117 (9)	0.0097 (10)

O2W	0.0368 (11)	0.0475 (12)	0.0960 (17)	−0.0007 (9)	0.0283 (11)	−0.0014 (12)
O3	0.0376 (10)	0.0508 (11)	0.0534 (11)	−0.0018 (9)	0.0205 (8)	0.0026 (9)
O4	0.0293 (9)	0.0504 (11)	0.0523 (11)	0.0028 (8)	0.0172 (8)	0.0012 (9)
C1	0.060 (2)	0.091 (3)	0.064 (2)	−0.0085 (19)	0.0011 (17)	−0.0121 (19)
C2	0.0413 (15)	0.0593 (18)	0.0526 (17)	0.0090 (14)	0.0065 (13)	−0.0069 (14)
C3	0.061 (2)	0.069 (2)	0.0494 (17)	−0.0020 (17)	0.0136 (15)	0.0018 (16)
C4	0.0449 (16)	0.0539 (17)	0.0573 (18)	0.0074 (14)	0.0198 (14)	0.0097 (14)
C5	0.072 (2)	0.088 (3)	0.075 (2)	−0.008 (2)	0.0251 (19)	0.023 (2)
C6	0.066 (2)	0.065 (2)	0.0618 (19)	−0.0130 (17)	0.0282 (16)	0.0053 (16)
C7	0.0377 (14)	0.0511 (17)	0.0449 (15)	−0.0059 (12)	0.0105 (11)	0.0021 (12)
C8	0.0567 (18)	0.0443 (16)	0.070 (2)	−0.0022 (14)	0.0236 (15)	−0.0010 (14)
C9	0.0352 (14)	0.0525 (17)	0.0547 (17)	0.0007 (13)	0.0078 (12)	−0.0051 (14)
C10	0.066 (2)	0.059 (2)	0.104 (3)	0.0101 (18)	0.040 (2)	−0.012 (2)
Cl1	0.0608 (5)	0.0566 (5)	0.0930 (7)	0.0043 (4)	0.0079 (4)	−0.0052 (5)
O5	0.121 (3)	0.087 (2)	0.115 (2)	−0.035 (2)	0.000 (2)	−0.0070 (18)
O6	0.173 (4)	0.198 (4)	0.139 (3)	−0.079 (4)	0.076 (3)	−0.095 (3)
O7	0.197 (4)	0.081 (2)	0.160 (4)	−0.048 (3)	0.000 (3)	0.008 (2)
O8	0.113 (3)	0.242 (5)	0.169 (4)	0.100 (4)	−0.016 (3)	−0.030 (4)
O3W	0.097 (2)	0.119 (2)	0.0580 (15)	−0.0363 (19)	−0.0006 (14)	0.0106 (16)

Geometric parameters (Å, °)

Cr1—O2	1.9306 (19)	C4—C5	1.499 (4)
Cr1—O3	1.9327 (19)	C5—H5A	0.96
Cr1—O4	1.9396 (19)	C5—H5B	0.96
Cr1—O1	1.947 (2)	C5—H5C	0.96
Cr1—O1W	1.991 (2)	C6—C7	1.496 (4)
Cr1—O2W	2.009 (2)	C6—H6A	0.96
O1—C2	1.291 (4)	C6—H6B	0.96
O1W—H1WA	0.833 (10)	C6—H6C	0.96
O1W—H1WB	0.829 (10)	C7—C8	1.379 (4)
O2—C4	1.272 (4)	C8—C9	1.387 (4)
O2W—H2WA	0.830 (10)	C8—H8	0.93
O2W—H2WB	0.839 (10)	C9—C10	1.483 (4)
O3—C7	1.269 (3)	C10—H10A	0.96
O4—C9	1.290 (3)	C10—H10B	0.96
C1—C2	1.502 (5)	C10—H10C	0.96
C1—H1A	0.96	Cl1—O6	1.348 (4)
C1—H1B	0.96	Cl1—O8	1.375 (4)
C1—H1C	0.96	Cl1—O5	1.421 (3)
C2—C3	1.376 (4)	Cl1—O7	1.430 (4)
C3—C4	1.389 (5)	O3W—H3WA	0.84 (4)
C3—H3	0.93	O3W—H3WB	0.84 (1)
O2—Cr1—O3	176.62 (8)	O2—C4—C3	123.9 (3)
O2—Cr1—O4	90.34 (8)	O2—C4—C5	115.3 (3)
O3—Cr1—O4	91.94 (8)	C3—C4—C5	120.8 (3)
O2—Cr1—O1	92.32 (9)	C4—C5—H5A	109.5
O3—Cr1—O1	90.21 (9)	C4—C5—H5B	109.5
O4—Cr1—O1	89.28 (8)	H5A—C5—H5B	109.5

O2—Cr1—O1W	86.96 (9)	C4—C5—H5C	109.5
O3—Cr1—O1W	90.49 (9)	H5A—C5—H5C	109.5
O4—Cr1—O1W	91.17 (9)	H5B—C5—H5C	109.5
O1—Cr1—O1W	179.15 (9)	C7—C6—H6A	109.5
O2—Cr1—O2W	91.26 (9)	C7—C6—H6B	109.5
O3—Cr1—O2W	86.51 (9)	H6A—C6—H6B	109.5
O4—Cr1—O2W	178.13 (8)	C7—C6—H6C	109.5
O1—Cr1—O2W	89.69 (10)	H6A—C6—H6C	109.5
O1W—Cr1—O2W	89.88 (10)	H6B—C6—H6C	109.5
C2—O1—Cr1	125.23 (19)	O3—C7—C8	124.3 (3)
Cr1—O1W—H1WA	119 (2)	O3—C7—C6	115.5 (3)
Cr1—O1W—H1WB	129 (2)	C8—C7—C6	120.2 (3)
H1WA—O1W—H1WB	111.2 (17)	C7—C8—C9	126.0 (3)
C4—O2—Cr1	126.8 (2)	C7—C8—H8	117.0
Cr1—O2W—H2WA	122 (2)	C9—C8—H8	117.0
Cr1—O2W—H2WB	128 (2)	O4—C9—C8	124.0 (3)
H2WA—O2W—H2WB	110.0 (17)	O4—C9—C10	114.5 (3)
C7—O3—Cr1	126.59 (18)	C8—C9—C10	121.4 (3)
C9—O4—Cr1	125.53 (17)	C9—C10—H10A	109.5
C2—C1—H1A	109.5	C9—C10—H10B	109.5
C2—C1—H1B	109.5	H10A—C10—H10B	109.5
H1A—C1—H1B	109.5	C9—C10—H10C	109.5
C2—C1—H1C	109.5	H10A—C10—H10C	109.5
H1A—C1—H1C	109.5	H10B—C10—H10C	109.5
H1B—C1—H1C	109.5	O6—Cl1—O8	113.7 (3)
O1—C2—C3	124.5 (3)	O6—Cl1—O5	112.4 (2)
O1—C2—C1	115.0 (3)	O8—Cl1—O5	109.0 (3)
C3—C2—C1	120.5 (3)	O6—Cl1—O7	110.5 (3)
C2—C3—C4	126.3 (3)	O8—Cl1—O7	104.7 (4)
C2—C3—H3	116.9	O5—Cl1—O7	106.1 (2)
C4—C3—H3	116.9	H3WB—O3W—H3WA	108 (2)
O2—Cr1—O1—C2	9.8 (2)	Cr1—O1—C2—C3	−6.5 (4)
O3—Cr1—O1—C2	−172.5 (2)	Cr1—O1—C2—C1	174.1 (2)
O4—Cr1—O1—C2	−80.6 (2)	O1—C2—C3—C4	−1.8 (5)
O2W—Cr1—O1—C2	101.0 (2)	C1—C2—C3—C4	177.6 (3)
O4—Cr1—O2—C4	80.5 (2)	Cr1—O2—C4—C3	4.3 (4)
O1—Cr1—O2—C4	−8.8 (2)	Cr1—O2—C4—C5	−176.3 (2)
O1W—Cr1—O2—C4	171.7 (2)	C2—C3—C4—O2	3.1 (5)
O2W—Cr1—O2—C4	−98.5 (2)	C2—C3—C4—C5	−176.3 (3)
O4—Cr1—O3—C7	−12.1 (2)	Cr1—O3—C7—C8	6.4 (4)
O1—Cr1—O3—C7	77.2 (2)	Cr1—O3—C7—C6	−174.8 (2)
O1W—Cr1—O3—C7	−103.3 (2)	O3—C7—C8—C9	3.7 (5)
O2W—Cr1—O3—C7	166.8 (2)	C6—C7—C8—C9	−175.1 (3)
O2—Cr1—O4—C9	−169.5 (2)	Cr1—O4—C9—C8	−8.3 (4)
O3—Cr1—O4—C9	13.0 (2)	Cr1—O4—C9—C10	172.3 (2)
O1—Cr1—O4—C9	−77.2 (2)	C7—C8—C9—O4	−2.5 (5)
O1W—Cr1—O4—C9	103.5 (2)	C7—C8—C9—C10	176.8 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O4^{i}	0.833 (10)	1.96 (2)	2.791 (3)	174 (3)
O1W—H1WB···O3W	0.829 (10)	1.79 (1)	2.616 (3)	171 (3)
O2W—H2WA···O1^{ii}	0.830 (10)	1.96 (2)	2.778 (3)	169 (3)
O2W—H2WB···O7	0.839 (10)	1.84 (1)	2.675 (4)	173 (4)
O3W—H3WA···O8^{iii}	0.84 (4)	1.96 (2)	2.770 (5)	161 (6)

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

Fig. 1

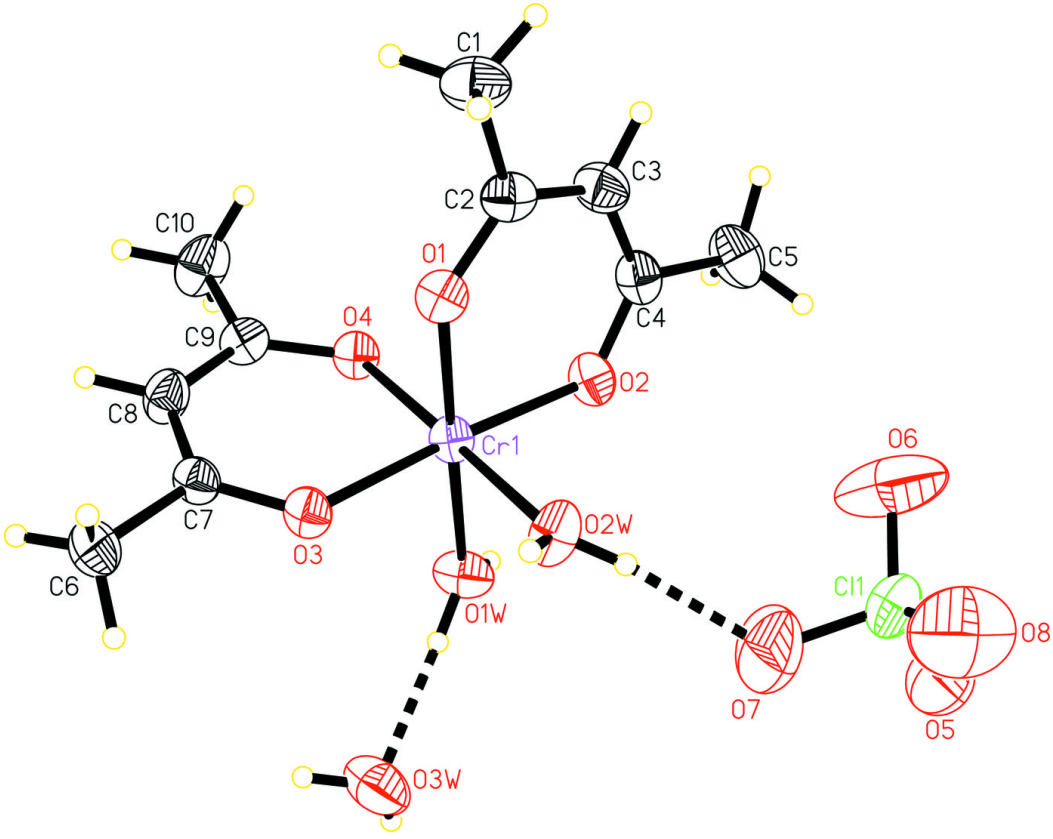
C1
C2
C3
C4
C5
C6
C7
C8
C9
C10
O1
O2
O3
O4
Cr1
O1W
O2W
O3W
Cl1
O5
O6
O7
O8

Fig. 2