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

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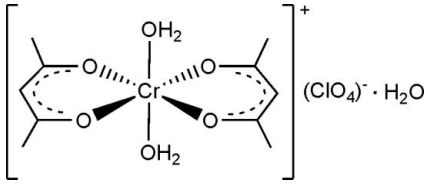
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.041; wR factor = 0.120; data-to-parameter ratio = 19.9.

Two crystallographically independent cations of the title complex, $[Cr(C_5H_7O_2)_2(H_2O)_2](ClO_4)\cdot H_2O$, are present in the asymmetric unit. Both cations are situated on centres of symmetry and share similar structural features. The geometry of the Cr^{3+} center is octahedral. The solvent water molecule and the perchlorate anion are involved in moderately strong hydrogen-bond interactions with the cations. In addition, neighboring cations are hydrogen-bonded together, resulting in a three-dimensional network.

Related literature

For synthesis, see: Ogino *et al.*, (1988); Arulsamy & Crawford (2007). For related structures, see: Arulsamy & Crawford (2007); 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
Triclinic, $P\overline{1}$
a = 8.4735 (1) Å
b = 10.1022 (1) Å
c = 10.3165 (1) Å
α = 91.925 (1)°
β = 98.254 (1)°
γ = 98.388 (1)°
V = 863.26 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.87 mm^{-1}
T = 296 (2) K
0.25 × 0.17 × 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004*a*)
T_{min} = 0.812, T_{max} = 0.899
8216 measured reflections
4395 independent reflections
3304 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.120
S = 1.06
4395 reflections
221 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cr1—O1	1.9378 (15)	Cr2—O3	1.9492 (18)
Cr1—O2	1.9398 (14)	Cr2—O4	1.9420 (14)
Cr1—O1*W*	2.0004 (15)	Cr2—O2*W*	1.9862 (16)
O1^{i}—Cr1—O1	180	O3^{ii}—Cr2—O3	180
O1—Cr1—O2^{i}	87.99 (7)	O4—Cr2—O3^{ii}	89.27 (7)
O1—Cr1—O2	92.01 (7)	O4—Cr2—O3	90.73 (7)
O2^{i}—Cr1—O2	180	O4—Cr2—O4^{ii}	180
O1^{i}—Cr1—O1*W*	90.44 (7)	O4—Cr2—O2*W*^{ii}	90.99 (7)
O1—Cr1—O1*W*	89.56 (7)	O4—Cr2—O2*W*	89.01 (7)
O2^{i}—Cr1—O1*W*	90.80 (6)	O3^{ii}—Cr2—O2*W*	90.15 (8)
O2—Cr1—O1*W*	89.20 (6)	O3—Cr2—O2*W*	89.85 (8)
O1*W*—Cr1—O1*W*^{i}	180	O2*W*^{ii}—Cr2—O2*W*	180

Symmetry codes: (i) $-x-1, -y+1, -z$; (ii) $-x+1, -y+2, -z+2$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*WA*···O3*W*	0.94	1.65	2.594 (3)	177
O1*W*—H1*WB*···O4^{iii}	0.86	1.98	2.832 (2)	171
O2*W*—H2*WA*···O2^{iv}	0.90	1.83	2.729 (2)	174
O2*W*—H2*WB*···O7	0.83	1.95	2.781 (3)	179
O3*W*—H3*WA*···O8^{iv}	0.83	2.20	3.008 (4)	162
O3*W*—H3*WB*···O6	0.89	2.03	2.908 (4)	173

Symmetry codes: (iii) $-x, -y+2, -z+1$; (iv) $-x, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HJ3062).

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  doi:10.1107/S1600536807059417

supplementary materials

Acta Cryst. (2007). E**63**, m3128 [**doi:10.1107/S1600536807059417**]

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

N. Arulsamy and J. L. Crawford

Comment

Our interest in Compound **I** stems from its usefulness as a starting material for the synthesis of mixed ligand (acetylacetonato)chromium(III)-amino acida complexes. We obtained crystals of **I** as a minor product together with the *cis* isomer from a modified literature procedure (Ogino *et al.*, 1988; Arulsamy & Crawford, 2007).

The asymmetric unit consists of two halves of the complex cation, a perchlorate anion, and a solvated water molecule. The Cr atoms of both cations are located on a twofold symmetry axis, whereas all atoms of the anion and the solvated water molecule are located on general positions. In both cations, two acetylacetonato ligands and two water molecules bind the Cr^{3+} center conferring a nearly perfect-octahedral geometry to the metal ion (Fig. 1). The Cr—O_{acac} bonds are only slightly shorter (*ca* 0.06 Å) than the two Cr—O_{aqua} bonds (Table 1)indicating strong bonds with the water molecules as observed in the *cis*-$[Cr(C_5H_7O_2)_2(H_2O)_2]^+$ (Arulsamy & Crawford, 2007), *trans*-bis(malonato)diaquachromium(III) (Lemmer *et al.*, 2002) and *cis*-bis(oxalato)diaquachromium(III) cations (Marinescu *et al.*, 2002). The constituents of the crystals of **I** are involved in moderately strong H-bonding interactions (Table 2). The axial water molecules of the cations are involved in mutual H-bonding interaction with neighboring cations through the chelating carboxylato O atoms. The axial water molecules of one of the crystallographically unique cations is strongly H-bonded to the solvated water molecules whereas the axial water molecules of the other cation is strongly H-bonded to the anionic O atoms resulting in a three-dimensional network (Fig. 2).

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; Arulsamy & Crawford, 2007). A brown-purple crystal of suitable size was chosen for the X-ray measurement.

Refinement

H atoms bonded to the water O atoms were located in successive difference maps and refined using a riding model with no changes being allowed to their positional parameters. The remaining H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93–0.96 Å and with U_{iso}(H) = 1.5 (1.2 for CH groups) times U_{eq}(C).

Figures

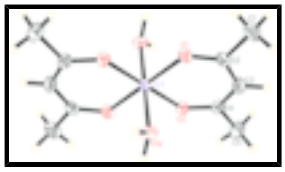

Fig. 1. Drawing of one of the unique *trans*-$[Cr(C_5H_7O_2)_2(H_2O)_2]^+$ cations with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are shown as small spheres with arbitrary radii.

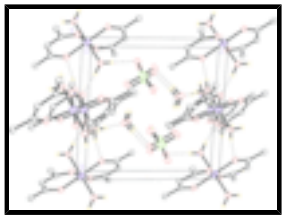

Fig. 2. The packing of **I** as viewed down the *a* axis.

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

Crystal data

$[Cr(C_5H_7O_2)_2(H_2O)_2](ClO_4)\cdot H_2O$	$Z = 2$
$M_r = 403.71$	$F_{000} = 418$
Triclinic, $P\overline{1}$	$D_x = 1.553$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.4735$ (1) Å	Cell parameters from 3912 reflections
$b = 10.1022$ (1) Å	$\theta = 2.8$–32.2°
$c = 10.3165$ (1) Å	$\mu = 0.87$ mm^{-1}
$\alpha = 91.925$ (1)°	$T = 296$ (2) K
$\beta = 98.254$ (1)°	Rectangular prism, purple
$\gamma = 98.388$ (1)°	0.25 × 0.17 × 0.13 mm
$V = 863.264$ (16) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	4395 independent reflections
Radiation source: fine-focus sealed tube	3304 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.027$
$T = 296(2)$ K	$\theta_{max} = 28.7^\circ$
phi and ω scans	$\theta_{min} = 2.0^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 2004a)	$h = -11 \rightarrow 11$
$T_{min} = 0.812$, $T_{max} = 0.899$	$k = -12 \rightarrow 13$
8216 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.120$	$w = 1/[\sigma^2(F_o^2) + (0.0604P)^2 + 0.1291P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.010$
4395 reflections	$\Delta\rho_{max} = 0.53$ e Å^{-3}
221 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2$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	−0.5000	0.5000	0.0000	0.02705 (13)
O1	−0.4718 (2)	0.57332 (16)	−0.16778 (15)	0.0375 (4)
O2	−0.32612 (18)	0.39562 (14)	−0.00618 (15)	0.0335 (3)
O1W	−0.33961 (19)	0.65211 (15)	0.08989 (16)	0.0378 (4)
H1WA	−0.2795	0.6354	0.1701	0.077 (11)*
H1WB	−0.3743	0.7268	0.0994	0.073 (11)*
C1	−0.3668 (4)	0.6284 (3)	−0.3601 (3)	0.0593 (8)
H1A	−0.3946	0.7161	−0.3463	0.089*
H1B	−0.4465	0.5778	−0.4257	0.089*
H1C	−0.2632	0.6365	−0.3888	0.089*
C2	−0.3609 (3)	0.5583 (2)	−0.2345 (2)	0.0367 (5)
C3	−0.2393 (3)	0.4799 (3)	−0.1982 (3)	0.0473 (6)
H3A	−0.1604	0.4794	−0.2522	0.057*
C4	−0.2265 (3)	0.4046 (2)	−0.0909 (2)	0.0353 (5)
C5	−0.0908 (3)	0.3242 (3)	−0.0624 (3)	0.0555 (7)
H5A	−0.1330	0.2358	−0.0401	0.083*
H5B	−0.0141	0.3673	0.0097	0.083*
H5C	−0.0385	0.3180	−0.1385	0.083*
Cr2	0.5000	1.0000	1.0000	0.02978 (14)
O3	0.7006 (2)	0.96239 (17)	0.94534 (17)	0.0435 (4)
O4	0.4621 (2)	1.11026 (14)	0.85140 (15)	0.0352 (4)
O2W	0.3801 (2)	0.84204 (16)	0.88978 (17)	0.0460 (4)

H2WA	0.3641	0.7608	0.9235	0.079 (11)*
H2WB	0.3463	0.8435	0.8102	0.069 (10)*
C6	0.9000 (4)	0.9363 (4)	0.8152 (3)	0.0700 (9)
H6A	0.8948	0.8430	0.8322	0.105*
H6B	0.9863	0.9876	0.8749	0.105*
H6C	0.9193	0.9492	0.7267	0.105*
C7	0.7446 (3)	0.9812 (2)	0.8333 (3)	0.0433 (6)
C8	0.6581 (4)	1.0418 (3)	0.7326 (3)	0.0476 (6)
H8A	0.6920	1.0396	0.6508	0.057*
C9	0.5269 (3)	1.1044 (2)	0.7444 (2)	0.0375 (5)
C10	0.4496 (4)	1.1741 (3)	0.6327 (3)	0.0545 (7)
H10A	0.3376	1.1364	0.6117	0.082*
H10B	0.5024	1.1628	0.5576	0.082*
H10C	0.4589	1.2678	0.6568	0.082*
Cl1	0.14280 (8)	0.74642 (7)	0.57605 (7)	0.05233 (19)
O5	0.1993 (5)	0.6524 (4)	0.4986 (4)	0.1280 (13)
O6	0.0140 (4)	0.7951 (4)	0.5022 (3)	0.1255 (13)
O7	0.2687 (4)	0.8519 (3)	0.6237 (3)	0.1001 (10)
O8	0.0877 (4)	0.6810 (3)	0.6845 (3)	0.0921 (8)
O3W	−0.1754 (3)	0.5970 (3)	0.3083 (2)	0.0835 (8)
H3WA	−0.1619	0.5190	0.3251	0.111 (16)*
H3WB	−0.1107	0.6558	0.3648	0.082 (12)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.0330 (3)	0.0250 (2)	0.0250 (2)	0.00974 (18)	0.00458 (18)	0.00419 (17)
O1	0.0456 (9)	0.0404 (9)	0.0293 (8)	0.0123 (7)	0.0071 (7)	0.0115 (7)
O2	0.0371 (8)	0.0307 (8)	0.0357 (8)	0.0123 (6)	0.0071 (6)	0.0053 (6)
O1W	0.0414 (9)	0.0296 (8)	0.0403 (9)	0.0083 (7)	−0.0034 (7)	−0.0007 (7)
C1	0.073 (2)	0.0684 (19)	0.0374 (15)	0.0051 (15)	0.0133 (13)	0.0176 (14)
C2	0.0439 (13)	0.0350 (11)	0.0285 (11)	−0.0031 (9)	0.0063 (9)	0.0004 (9)
C3	0.0441 (14)	0.0573 (16)	0.0450 (15)	0.0108 (12)	0.0178 (11)	0.0045 (12)
C4	0.0321 (11)	0.0317 (11)	0.0420 (13)	0.0050 (9)	0.0061 (9)	−0.0029 (9)
C5	0.0413 (14)	0.0515 (15)	0.078 (2)	0.0177 (12)	0.0128 (13)	0.0058 (14)
Cr2	0.0447 (3)	0.0222 (2)	0.0219 (2)	0.00884 (19)	−0.00079 (19)	0.00258 (17)
O3	0.0531 (10)	0.0452 (10)	0.0355 (9)	0.0209 (8)	0.0038 (7)	0.0046 (7)
O4	0.0526 (10)	0.0282 (7)	0.0257 (8)	0.0116 (7)	0.0023 (7)	0.0057 (6)
O2W	0.0737 (12)	0.0270 (8)	0.0307 (9)	0.0025 (8)	−0.0093 (8)	0.0027 (7)
C6	0.064 (2)	0.093 (2)	0.060 (2)	0.0358 (18)	0.0097 (15)	−0.0072 (18)
C7	0.0515 (14)	0.0404 (13)	0.0381 (13)	0.0089 (11)	0.0064 (11)	−0.0043 (10)
C8	0.0635 (17)	0.0519 (15)	0.0300 (12)	0.0140 (13)	0.0097 (11)	0.0021 (11)
C9	0.0550 (14)	0.0294 (11)	0.0261 (11)	0.0039 (10)	0.0012 (10)	0.0052 (9)
C10	0.078 (2)	0.0576 (16)	0.0305 (13)	0.0194 (14)	0.0052 (12)	0.0155 (12)
Cl1	0.0531 (4)	0.0576 (4)	0.0407 (4)	0.0015 (3)	−0.0030 (3)	−0.0046 (3)
O5	0.125 (3)	0.136 (3)	0.124 (3)	0.016 (2)	0.043 (2)	−0.060 (2)
O6	0.127 (3)	0.117 (2)	0.117 (3)	0.036 (2)	−0.053 (2)	0.011 (2)
O7	0.124 (2)	0.0891 (18)	0.0598 (15)	−0.0469 (17)	−0.0152 (15)	0.0045 (14)

O8	0.098 (2)	0.0925 (19)	0.0856 (19)	−0.0049 (15)	0.0306 (15)	0.0158 (15)
O3W	0.0992 (19)	0.0619 (15)	0.0730 (16)	0.0137 (13)	−0.0441 (14)	0.0041 (12)

Geometric parameters (Å, °)

Cr1—O1^{i}	1.9378 (15)	Cr2—O4^{ii}	1.9420 (14)
Cr1—O1	1.9378 (15)	Cr2—O2W^{ii}	1.9862 (16)
Cr1—O2^{i}	1.9398 (14)	Cr2—O2W	1.9862 (16)
Cr1—O2	1.9398 (14)	O3—C7	1.276 (3)
Cr1—O1W	2.0004 (15)	O4—C9	1.305 (3)
Cr1—O1W^{i}	2.0004 (15)	O2W—H2WA	0.9013
O1—C2	1.264 (3)	O2W—H2WB	0.8315
O2—C4	1.296 (3)	C6—C7	1.488 (4)
O1W—H1WA	0.9413	C6—H6A	0.9600
O1W—H1WB	0.8568	C6—H6B	0.9600
C1—C2	1.496 (3)	C6—H6C	0.9600
C1—H1A	0.9600	C7—C8	1.395 (4)
C1—H1B	0.9600	C8—C9	1.375 (4)
C1—H1C	0.9600	C8—H8A	0.9300
C2—C3	1.406 (4)	C9—C10	1.492 (3)
C3—C4	1.364 (4)	C10—H10A	0.9600
C3—H3A	0.9300	C10—H10B	0.9600
C4—C5	1.504 (3)	C10—H10C	0.9600
C5—H5A	0.9600	Cl1—O6	1.399 (3)
C5—H5B	0.9600	Cl1—O5	1.401 (3)
C5—H5C	0.9600	Cl1—O7	1.413 (2)
Cr2—O3^{ii}	1.9492 (18)	Cl1—O8	1.420 (3)
Cr2—O3	1.9492 (18)	O3W—H3WA	0.8328
Cr2—O4	1.9420 (14)	O3W—H3WB	0.8855
O1^{i}—Cr1—O1	180.00 (9)	O4^{ii}—Cr2—O3	89.27 (7)
O1^{i}—Cr1—O2^{i}	92.01 (7)	O4—Cr2—O4^{ii}	180.000 (1)
O1—Cr1—O2^{i}	87.99 (7)	O4—Cr2—O2W^{ii}	90.99 (7)
O1^{i}—Cr1—O2	87.99 (7)	O4^{ii}—Cr2—O2W^{ii}	89.01 (7)
O1—Cr1—O2	92.01 (7)	O3^{ii}—Cr2—O2W^{ii}	89.85 (8)
O2^{i}—Cr1—O2	180.0	O3—Cr2—O2W^{ii}	90.15 (8)
O1^{i}—Cr1—O1W	90.44 (7)	O4—Cr2—O2W	89.01 (7)
O1—Cr1—O1W	89.56 (7)	O4^{ii}—Cr2—O2W	90.99 (7)
O2^{i}—Cr1—O1W	90.80 (6)	O3^{ii}—Cr2—O2W	90.15 (8)
O2—Cr1—O1W	89.20 (6)	O3—Cr2—O2W	89.85 (8)
O1^{i}—Cr1—O1W^{i}	89.56 (7)	O2W^{ii}—Cr2—O2W	180.0
O1—Cr1—O1W^{i}	90.44 (7)	C7—O3—Cr2	126.76 (16)
O2^{i}—Cr1—O1W^{i}	89.20 (6)	C9—O4—Cr2	125.35 (14)
O2—Cr1—O1W^{i}	90.80 (6)	Cr2—O2W—H2WA	120.7
O1W—Cr1—O1W^{i}	180.0	Cr2—O2W—H2WB	124.1
C2—O1—Cr1	126.92 (15)	H2WA—O2W—H2WB	115.1

C4—O2—Cr1	125.96 (14)	C7—C6—H6A	109.5
Cr1—O1W—H1WA	116.9	C7—C6—H6B	109.5
Cr1—O1W—H1WB	116.3	H6A—C6—H6B	109.5
H1WA—O1W—H1WB	108.2	C7—C6—H6C	109.5
C2—C1—H1A	109.5	H6A—C6—H6C	109.5
C2—C1—H1B	109.5	H6B—C6—H6C	109.5
H1A—C1—H1B	109.5	O3—C7—C8	124.0 (2)
C2—C1—H1C	109.5	O3—C7—C6	115.7 (2)
H1A—C1—H1C	109.5	C8—C7—C6	120.3 (3)
H1B—C1—H1C	109.5	C9—C8—C7	125.3 (2)
O1—C2—C3	124.1 (2)	C9—C8—H8A	117.4
O1—C2—C1	115.6 (2)	C7—C8—H8A	117.4
C3—C2—C1	120.2 (2)	O4—C9—C8	124.1 (2)
C4—C3—C2	125.9 (2)	O4—C9—C10	114.9 (2)
C4—C3—H3A	117.1	C8—C9—C10	121.0 (2)
C2—C3—H3A	117.1	C9—C10—H10A	109.5
O2—C4—C3	124.4 (2)	C9—C10—H10B	109.5
O2—C4—C5	114.5 (2)	H10A—C10—H10B	109.5
C3—C4—C5	121.1 (2)	C9—C10—H10C	109.5
C4—C5—H5A	109.5	H10A—C10—H10C	109.5
C4—C5—H5B	109.5	H10B—C10—H10C	109.5
H5A—C5—H5B	109.5	O6—Cl1—O5	109.4 (2)
C4—C5—H5C	109.5	O6—Cl1—O7	111.0 (2)
H5A—C5—H5C	109.5	O5—Cl1—O7	110.3 (2)
H5B—C5—H5C	109.5	O6—Cl1—O8	109.1 (2)
$O3^{ii}$—Cr2—O3	180.000 (1)	O5—Cl1—O8	108.2 (2)
O4—Cr2—$O3^{ii}$	89.27 (7)	O7—Cl1—O8	108.72 (17)
$O4^{ii}$—Cr2—$O3^{ii}$	90.73 (7)	H3WA—O3W—H3WB	110.8
O4—Cr2—O3	90.73 (7)		

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1W—H1WA···O3W	0.94	1.65	2.594 (3)	177
O1W—H1WB···$O4^{iii}$	0.86	1.98	2.832 (2)	171
O2W—H2WA···$O2^{iv}$	0.90	1.83	2.729 (2)	174
O2W—H2WB···O7	0.83	1.95	2.781 (3)	179
O3W—H3WA···$O8^{iv}$	0.83	2.20	3.008 (4)	162
O3W—H3WB···O6	0.89	2.03	2.908 (4)	173

Symmetry codes: (iii) −*x*, −*y*+2, −*z*+1; (iv) −*x*, −*y*+1, −*z*+1.

Fig. 1

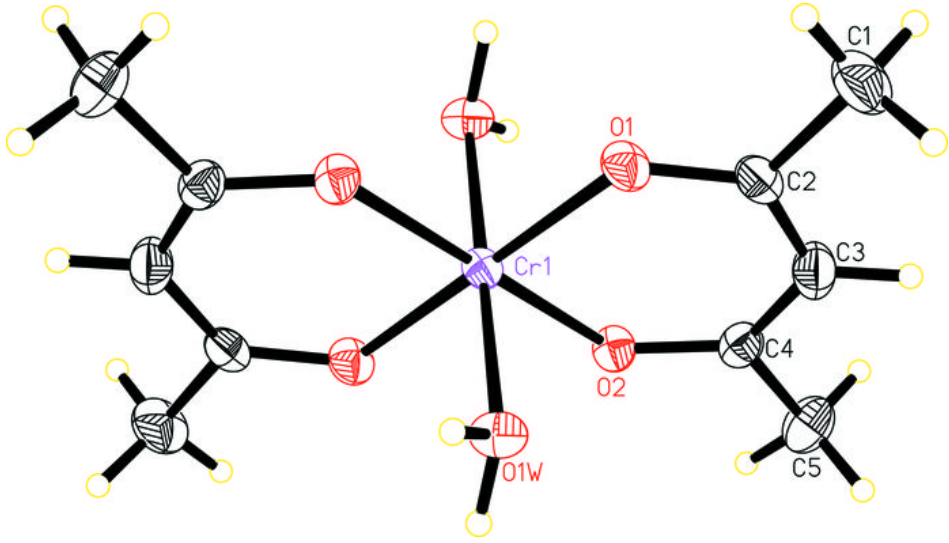

Fig. 2