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(Oxalato-κ^2O,O')bis(propane-1,3-diamine-κ^2N,N')chromium(III) chloride monohydrate

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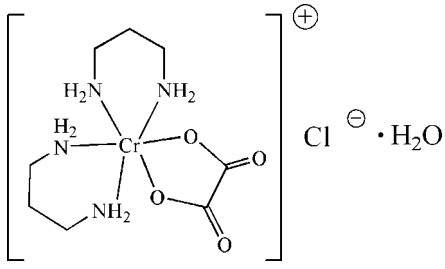
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.027; wR factor = 0.071; data-to-parameter ratio = 8.9.

The asymmetric unit of the title monohydrated salt, $[Cr(C_2O_4)(C_3H_{10}N_2)_2]Cl\cdot H_2O$, contains two formula units. The Cr atom is chelated by the oxalate dianions in an octahedral geometry. Hydrogen bonds involving the N atoms of the ligands, the O atoms of the oxalate group, the chloride anion and the solvent water molecule connect the components into a three-dimensional network structure.

Related literature

For bis(oxalato)chromates, see: Bruda *et al.* (2001); De Munno *et al.* (1999); Lescouëzec *et al.* (2003); Sakagami *et al.* (1999). For mono(oxalato)chromates, see: Marinescu *et al.* (2000). For a chromium complex with an oxalate group in both the cation and anion, see: Lethbridge *et al.* (1970). For the synthesis of a precursor to the title compound, see: Pedersen (1970).



Experimental

Crystal data

$[Cr(C_2O_4)(C_3H_{10}N_2)_2]Cl\cdot H_2O$
M_r = 341.74
Monoclinic, *Pn*
a = 8.9532 (17) Å
b = 12.038 (2) Å
c = 13.645 (3) Å
β = 99.973 (14)°
V = 1448.5 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.00 mm^{-1}
T = 293 (2) K
0.30 × 0.25 × 0.10 mm

Data collection

Bruker *P*4 diffractometer
Absorption correction: ψ-scan (North *et al.*, 1968)
T_{min} = 0.742, T_{max} = 0.905
3397 measured reflections
3084 independent reflections
3056 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
3 standard reflections
every 97 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.027
$wR(F^2)$ = 0.071
S = 1.00
3084 reflections
348 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Flack (1983), with 526 Friedel pairs
Flack parameter: 0.017 (15)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···Cl2^{i}	0.90	2.46	3.353 (4)	172
N4—H4D···O3^{ii}	0.90	2.02	2.913 (4)	175
N7—H7A···O7^{iii}	0.90	2.12	2.994 (5)	164
N7—H7B···Cl2	0.90	2.54	3.323 (4)	145
N1—H1A···O7^{iv}	0.90	2.16	3.047 (4)	170
N1—H1D···O3^{ii}	0.90	2.39	3.141 (5)	141
N5—H5A···O6^{iii}	0.90	1.97	2.780 (4)	149
N5—H5D···Cl1	0.90	2.28	3.160 (4)	165
N8—H8A···Cl2^{v}	0.90	2.50	3.329 (3)	154
N8—H8B···Cl1	0.90	2.69	3.383 (4)	135
N3—H3A···O7^{iv}	0.90	2.23	3.064 (4)	155
N3—H3D···O2W	0.90	2.15	3.000 (4)	157
N6—H6A···O1^{vi}	0.90	2.47	3.248 (4)	145
N6—H6D···Cl2	0.90	2.47	3.360 (3)	171
N2—H2A···O2^{ii}	0.90	2.53	3.363 (4)	154
N2—H2D···Cl1^{vii}	0.90	2.56	3.323 (3)	143
O1W—H100···Cl1	0.85	2.47	3.169 (4)	140
O1W—H101···O5	0.85	2.29	3.082 (5)	154
O2W—H200···Cl2^{iv}	0.85	2.49	3.298 (4)	160
O2W—H201···O1W^{iii}	0.85	1.95	2.800 (4)	173

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

Data collection: *XSCANS* (Bruker, 1997); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1998); software used to prepare material for publication: *SHELXL97* and *XP*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2312).

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supplementary materials

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(Oxalato-κ^2O,O')bis(propane-1,3-diamine-κ^2N,N')chromium(III) chloride monohydrate

L.-F. Zhang, J.-Y. Kou and H.-Z. Kou

Comment

The crystal structures of monomeric chromium(III) complexes $Na[Cr(hm)(ox)_2]\cdot 3H_2O$ (hm = histamine) and $Na[Cr(PM)(ox)_2]\cdot H_2O$ (PM = pyridoxamine) (Sakagami *et al.*, 1999), $AsPh_4[Cr(ox)(phen)]\cdot H_2O$ and $[NaCr(phen)(ox)_2(H_2O)]\cdot 2H_2O$ (phen = 1,10-phenanthroline) (Marinescu *et al.*, 2000), $AsPh_4[Cr(bpm)(ox)_2]\cdot H_2O$ and $Na[Cr(bpm)(ox)_2]\cdot H_2O$ (bpm = 2,2'-bipyrimidine) (De Munno *et al.*, 1999), and $PPh_4[Cr(bipy)(ox)_2]\cdot H_2O$ (bipy = 2,2'-bipyridine) (Lescouëzec *et al.*, 2003) contain two oxalato ligands and one neutral didentate terminal ligand. Among these examples, the complexes using the Na^+ ion as balanced anions usually show beautiful one-, two- or three-dimensional supramolecular structures. The compound [Mn(4,4'-bipyridine-*N*,*N*'- dioxide)$(H_2O)_4$][Cr(bipy)$(ox)_2]_2\cdot 8H_2O$ comprises of $[Cr(bipy)(ox)_2]^-$ anions and one-dimensional cationic chain $[Mn(4,4'\text{-bipyridine-}N,N'\text{- dioxide})(H_2O)_4]_n^{2n+}$ (Bruda *et al.*, 2001). The molecular structure of $[Cr(en)_2(ox)][Cr(en)(ox)_2]\cdot 2H_2O$ (en = 1,2-ethylenediamine) consists of one $[Cr(en)_2(ox)]^+$ cation and one $[Cr(en)(ox)_2]^-$ anion with one and two oxalato ligands, respectivley (Lethbridge *et al.*, 1970). Herein we report a new monooxalato-containing chromium(III) complex $[Cr(ox)(tn)_2]Cl\cdot H_2O$ (I).

The crystal structure of (I) consists of two independent $[Cr(tn)_2(ox)]^+$ cations, two free Cl^- as counteranions and two crystallization water molecules. (Figure 1). Each chromium atom in (I) is coordinated by four nitrogen atoms from two tn ligands and two oxalate oxygen atoms, yielding a distorted octahedral geometry. The four Cr—O bond distances (1.957 (2) to 1.994 (2) Å) are comparable to those in $[Cr(en)_2(ox)]^+$ unit of complex $[Cr(en)_2(ox)][Cr(en)(ox)_2]\cdot 2H_2O$. The Cr—N distances range from 2.063 (3) to 2.101 (3) Å for Cr1, and from 2.048 (3) to 2.093 (3) Å for Cr2. The bond angles between every adjacent two bonds around Cr atom are almost all close to 90 ° except O4—Cr1—O1 (82.30 (9) °) and O5—Cr2—O8 (82.47 (10) °), which leads to the distortion of coordination environment from the ideal octahedron. The ox ligands exhibit slightly deviation from planarity and the tn ligands show the typical chair-like conformation. The nearest Cr1···Cr2 separation is 6.061 Å.

There exist affluent hydrogen bonds in (I) (Figure 2). Firstly, the adjacent the adjacent two $[Cr1(tn)_2(ox)]^+$ units are linked by three N—H···O (N4—H4D···O3 [$x + 1/2, -y + 2, z + 1/2$], N1—H1D···O3 [$x + 1/2, -y + 2, z + 1/2$] and N2—H2A···O2 [$x + 1/2, -y + 2, z + 1/2$]) hydrogen bonds. Similarly, two $[Cr2(tn)_2(ox)]^+$ units are linked with two strong N—H···O (N5—H5A···O6 [$x - 1/2, -y + 1, z - 1/2$] and N7—H7A···O7 [$x - 1/2, -y + 1, z - 1/2$]) hydrogen bonds. Secondly, there are also three N—H···O (N1—H1A···O7 [$x - 1, y, z$], N3—H3A···O7 [$x - 1, y, z$], N6—H6A···O1 [$x + 1, y, z$]) hydrogen bonds between the nearest $[Cr1(tn)_2(ox)]^+$ and $[Cr2(tn)_2(ox)]^+$ units. Through all these N—H···O hydrogen bonds and seven N—H··· Cl hydrogen bonds, the two $[Cr(tn)_2(ox)]^+$ cationic units form two-dimensional layer-like structures. Finally, the layers form a three-dimensional network structure through hydrogen bond series N3···O2W···O1W [$x - 1/2, -y + 1, z - 1/2$]···O5 and two O_{water}···Cl hydrogen bonds.

Experimental

To a stirred aqueous solution (45 ml) of *cis*-$[Cr(tn)_2Cl_2]Cl$ (Pedersen, 1970) (2.4 g, 7.8 mmol) were slowly added $H_2C_2O_4{\cdot}2H_2O$ (1.2 g, 9.5 mmol) in 40 ml water. The solution was filtered and evaporated at room temperature. Orange crystal formed after about two weeks. Yield: 20%.

Refinement

The coordinates of the H atoms of the water molecules were found from difference Fourier maps. H atoms bound to C and N atoms were also visible in difference maps and were placed using the HFIX commands in *SHELXL97*. All H atoms were allowed for as riding atoms (C—H 0.97 Å, N—H 0.90 Å, O—H 0.85 Å) with the constraint $U(H) = 1.2U_{eq}$(carrier) for all other H atoms. The Flack parameter refined to 0.017 (15) from 526 Friedel pairs (Flack, 1983).

Figures

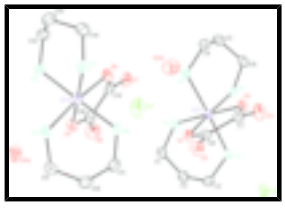

Fig. 1. A view of (I) with the unique atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. All H atoms have been omitted.

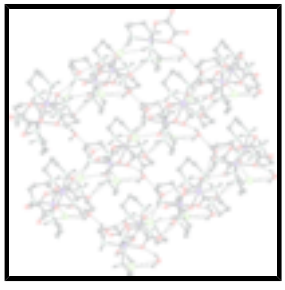

Fig. 2. The hydrogen-bonded sheet structure present in (I) along the *b* axis. H atoms bonded to C atoms have been omitted.

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Crystal data

$[Cr(C_2O_4)(C_3H_{10}N_2)_2]Cl{\cdot}H_2O$	F_{000} = 716
M_r = 341.74	D_x = 1.567 Mg m^{-3}
Monoclinic, *Pn*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: P -2yac	Cell parameters from 25 reflections
a = 8.9532 (17) Å	θ = 10.5–15.4º
b = 12.038 (2) Å	μ = 1.00 mm^{-1}
c = 13.645 (3) Å	*T* = 293 (2) K
β = 99.973 (14)º	Block, orange
V = 1448.5 (5) Å^3	0.30 × 0.25 × 0.10 mm
Z = 4	

Data collection

Bruker P4 diffractometer	R_{int} = 0.023
Radiation source: fine-focus sealed tube	θ_{max} = 25.0º
Monochromator: graphite	θ_{min} = 2.3º
T = 293(2) K	h = −1→10
ω scans	k = −14→1
Absorption correction: ψ scan (North *et al.*, 1968)	l = −16→16
T_{min} = 0.742, T_{max} = 0.905	3 standard reflections
3397 measured reflections	every 97 reflections
3084 independent reflections	intensity decay: none
3056 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.027	$w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 0.2592P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.071	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.00	$\Delta\rho_{max}$ = 0.45 e Å^{-3}
3084 reflections	$\Delta\rho_{min}$ = −0.34 e Å^{-3}
348 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
2 restraints	Extinction coefficient: 0.0164 (14)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), with 526 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.017 (15)

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 $F^2 > \sigma(F^2)$ 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	0.11216 (5)	0.95504 (3)	0.50724 (3)	0.02451 (13)
Cr2	0.91647 (5)	0.49199 (4)	0.36494 (3)	0.02758 (13)
Cl1	0.72903 (10)	0.17592 (7)	0.40994 (7)	0.0437 (2)
Cl2	0.72668 (12)	0.69845 (7)	0.10465 (7)	0.0501 (2)
O8	1.1124 (3)	0.56581 (19)	0.42017 (17)	0.0377 (5)
O4	0.0934 (3)	1.05364 (16)	0.39174 (16)	0.0315 (5)
O1	−0.0788 (3)	0.89196 (18)	0.43131 (16)	0.0311 (4)
O3	−0.0479 (3)	1.0854 (2)	0.24315 (17)	0.0447 (6)
N4	0.3109 (3)	1.0355 (2)	0.56628 (19)	0.0302 (6)
H4A	0.2864	1.1045	0.5831	0.036*
H4D	0.3507	1.0003	0.6230	0.036*
O6	1.0014 (4)	0.5508 (3)	0.65332 (19)	0.0585 (8)
O2	−0.2401 (3)	0.9151 (2)	0.28784 (18)	0.0416 (6)
O5	0.8982 (3)	0.48382 (19)	0.50579 (16)	0.0372 (5)
C7	−0.0216 (4)	1.0350 (3)	0.3227 (2)	0.0326 (7)
N7	0.9481 (4)	0.4989 (2)	0.2183 (2)	0.0388 (7)
H7A	0.8791	0.4541	0.1822	0.047*
H7B	0.9280	0.5686	0.1962	0.047*
N1	0.1263 (3)	0.8508 (2)	0.63199 (18)	0.0321 (5)
H1A	0.1693	0.7863	0.6184	0.038*
H1D	0.1883	0.8828	0.6832	0.038*
N5	0.7049 (3)	0.4228 (2)	0.3303 (2)	0.0343 (6)
H5A	0.6725	0.4323	0.2646	0.041*
H5D	0.7145	0.3492	0.3411	0.041*
N8	1.0256 (3)	0.3378 (2)	0.3778 (2)	0.0337 (6)
H8A	1.0494	0.3217	0.4430	0.040*
H8B	0.9579	0.2866	0.3502	0.040*
C16	1.0020 (5)	0.5343 (3)	0.5649 (2)	0.0386 (8)
N3	0.2297 (3)	0.8394 (2)	0.43456 (18)	0.0313 (5)
H3A	0.2635	0.7852	0.4782	0.038*
H3D	0.1630	0.8083	0.3853	0.038*
O7	1.2405 (3)	0.6304 (2)	0.5638 (2)	0.0460 (6)
N6	0.8089 (3)	0.6469 (2)	0.3501 (2)	0.0353 (6)
H6A	0.8791	0.6992	0.3713	0.042*
H6D	0.7756	0.6591	0.2849	0.042*
N2	−0.0082 (3)	1.0630 (2)	0.58323 (19)	0.0332 (6)
H2A	0.0574	1.0935	0.6334	0.040*
H2D	−0.0444	1.1184	0.5414	0.040*
C4	0.3594 (4)	0.8806 (3)	0.3915 (2)	0.0375 (7)
H4B	0.3233	0.9340	0.3396	0.045*
H4C	0.4046	0.8190	0.3613	0.045*
C5	0.4799 (4)	0.9351 (3)	0.4691 (3)	0.0417 (8)
H5B	0.5050	0.8853	0.5254	0.050*
H5C	0.5709	0.9459	0.4407	0.050*
C8	−0.1270 (4)	0.9398 (3)	0.3463 (2)	0.0303 (6)
C11	0.6798 (5)	0.6637 (3)	0.4033 (3)	0.0442 (8)
H11A	0.6455	0.7401	0.3950	0.053*
H11B	0.7131	0.6504	0.4738	0.053*
C1	−0.0201 (4)	0.8257 (3)	0.6641 (2)	0.0367 (7)

H1B	−0.0043	0.7693	0.7156	0.044*
H1C	−0.0907	0.7962	0.6081	0.044*
C9	0.5841 (4)	0.4639 (3)	0.3831 (3)	0.0432 (8)
H9A	0.6153	0.4518	0.4540	0.052*
H9B	0.4924	0.4213	0.3615	0.052*
C12	1.1642 (4)	0.3234 (3)	0.3342 (3)	0.0438 (8)
H12A	1.2000	0.2476	0.3450	0.053*
H12B	1.2426	0.3724	0.3678	0.053*
C6	0.4317 (4)	1.0457 (3)	0.5058 (3)	0.0393 (8)
H6B	0.5191	1.0814	0.5453	0.047*
H6C	0.3961	1.0930	0.4490	0.047*
C2	−0.0870 (4)	0.9273 (3)	0.7031 (3)	0.0413 (8)
H2B	−0.0125	0.9592	0.7556	0.050*
H2C	−0.1739	0.9052	0.7322	0.050*
C3	−0.1370 (4)	1.0163 (3)	0.6254 (3)	0.0383 (7)
H3B	−0.2104	0.9847	0.5720	0.046*
H3C	−0.1866	1.0757	0.6555	0.046*
C10	0.5496 (5)	0.5868 (3)	0.3646 (3)	0.0497 (9)
H10A	0.5201	0.5986	0.2936	0.060*
H10B	0.4637	0.6066	0.3957	0.060*
C14	1.1000 (5)	0.4677 (3)	0.1975 (3)	0.0495 (9)
H14A	1.1761	0.5151	0.2359	0.059*
H14B	1.1026	0.4797	0.1276	0.059*
C15	1.1322 (4)	0.5803 (2)	0.5151 (3)	0.0368 (7)
C13	1.1372 (6)	0.3483 (3)	0.2232 (3)	0.0527 (10)
H13A	1.2274	0.3279	0.1969	0.063*
H13B	1.0546	0.3021	0.1906	0.063*
O2W	0.0565 (4)	0.7737 (3)	0.2347 (2)	0.0611 (8)
O1W	0.7699 (6)	0.2955 (3)	0.6197 (3)	0.0797 (11)
H100	0.7126	0.2699	0.5685	0.26 (7)*
H101	0.8291	0.3453	0.6044	0.14 (3)*
H200	−0.0276	0.7710	0.1948	0.10 (2)*
H201	0.1253	0.7580	0.2011	0.067 (15)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.0265 (2)	0.0242 (2)	0.0218 (2)	−0.00091 (18)	0.00145 (16)	0.00035 (17)
Cr2	0.0303 (2)	0.0263 (2)	0.0242 (2)	−0.0022 (2)	−0.00081 (18)	0.00103 (16)
Cl1	0.0445 (4)	0.0343 (4)	0.0525 (5)	0.0006 (4)	0.0088 (4)	0.0070 (3)
Cl2	0.0647 (6)	0.0367 (4)	0.0416 (4)	−0.0017 (4)	−0.0112 (4)	0.0025 (3)
O8	0.0386 (13)	0.0371 (11)	0.0346 (12)	−0.0069 (11)	−0.0010 (10)	0.0013 (9)
O4	0.0356 (12)	0.0309 (10)	0.0255 (10)	−0.0042 (9)	−0.0018 (9)	0.0028 (8)
O1	0.0329 (11)	0.0302 (9)	0.0284 (9)	−0.0042 (9)	0.0002 (9)	−0.0004 (8)
O3	0.0547 (15)	0.0454 (13)	0.0288 (11)	−0.0061 (12)	−0.0068 (11)	0.0104 (10)
N4	0.0295 (14)	0.0301 (13)	0.0290 (13)	−0.0015 (11)	−0.0002 (11)	−0.0013 (10)
O6	0.071 (2)	0.0729 (19)	0.0276 (12)	−0.0007 (16)	−0.0035 (13)	−0.0113 (11)
O2	0.0380 (14)	0.0455 (13)	0.0372 (12)	−0.0049 (11)	−0.0047 (11)	−0.0032 (10)

O5	0.0426 (14)	0.0399 (11)	0.0275 (11)	−0.0033 (11)	0.0013 (10)	0.0037 (9)
C7	0.0361 (18)	0.0323 (15)	0.0284 (15)	0.0022 (13)	0.0027 (14)	−0.0010 (12)
N7	0.0513 (19)	0.0346 (14)	0.0296 (14)	0.0042 (13)	0.0042 (13)	0.0025 (10)
N1	0.0376 (14)	0.0307 (12)	0.0271 (12)	0.0004 (11)	0.0036 (11)	0.0003 (10)
N5	0.0342 (15)	0.0298 (12)	0.0353 (13)	−0.0013 (12)	−0.0045 (11)	0.0033 (10)
N8	0.0343 (13)	0.0307 (12)	0.0344 (13)	−0.0013 (12)	0.0011 (11)	0.0044 (10)
C16	0.047 (2)	0.0335 (15)	0.0320 (17)	0.0050 (15)	−0.0020 (15)	0.0018 (13)
N3	0.0369 (14)	0.0280 (11)	0.0287 (12)	−0.0016 (12)	0.0053 (11)	−0.0004 (10)
O7	0.0457 (14)	0.0331 (12)	0.0506 (13)	−0.0035 (11)	−0.0155 (12)	−0.0003 (10)
N6	0.0403 (15)	0.0284 (12)	0.0351 (13)	−0.0018 (11)	0.0006 (12)	0.0004 (10)
N2	0.0369 (15)	0.0298 (12)	0.0322 (13)	0.0016 (11)	0.0040 (12)	0.0004 (10)
C4	0.0375 (17)	0.0385 (16)	0.0389 (16)	0.0003 (14)	0.0134 (14)	−0.0021 (13)
C5	0.0332 (18)	0.0469 (18)	0.0454 (18)	0.0006 (16)	0.0078 (15)	0.0000 (15)
C8	0.0313 (16)	0.0316 (13)	0.0266 (14)	−0.0004 (13)	0.0016 (13)	−0.0035 (11)
C11	0.049 (2)	0.0338 (16)	0.0510 (19)	0.0076 (16)	0.0115 (17)	−0.0059 (14)
C1	0.0423 (18)	0.0338 (15)	0.0348 (15)	−0.0048 (14)	0.0089 (15)	0.0045 (13)
C9	0.0368 (19)	0.047 (2)	0.0461 (19)	−0.0057 (16)	0.0089 (16)	0.0002 (15)
C12	0.0383 (18)	0.0419 (18)	0.0520 (19)	0.0068 (16)	0.0099 (16)	0.0086 (15)
C6	0.0373 (18)	0.0417 (18)	0.0394 (17)	−0.0108 (15)	0.0082 (15)	−0.0026 (13)
C2	0.0440 (19)	0.0444 (18)	0.0372 (17)	0.0018 (16)	0.0119 (16)	0.0037 (14)
C3	0.0377 (18)	0.0414 (17)	0.0373 (17)	0.0040 (15)	0.0101 (15)	−0.0009 (13)
C10	0.0367 (18)	0.051 (2)	0.060 (2)	0.0076 (17)	0.0059 (17)	−0.0041 (18)
C14	0.061 (3)	0.048 (2)	0.043 (2)	0.0012 (19)	0.0209 (19)	0.0090 (16)
C15	0.0379 (18)	0.0253 (13)	0.0420 (18)	0.0022 (14)	−0.0076 (15)	−0.0009 (14)
C13	0.067 (3)	0.045 (2)	0.052 (2)	0.0142 (19)	0.027 (2)	0.0023 (17)
O2W	0.0577 (18)	0.081 (2)	0.0442 (14)	0.0030 (16)	0.0067 (14)	−0.0099 (14)
O1W	0.118 (3)	0.0555 (18)	0.077 (2)	−0.015 (2)	0.048 (2)	−0.0022 (16)

Geometric parameters (Å, °)

Cr1—O4	1.957 (2)	N6—H6A	0.9000
Cr1—O1	1.990 (2)	N6—H6D	0.9000
Cr1—N4	2.063 (3)	N2—C3	1.486 (5)
Cr1—N2	2.077 (3)	N2—H2A	0.9000
Cr1—N3	2.095 (3)	N2—H2D	0.9000
Cr1—N1	2.101 (3)	C4—C5	1.523 (5)
Cr2—O5	1.959 (2)	C4—H4B	0.9700
Cr2—O8	1.994 (2)	C4—H4C	0.9700
Cr2—N5	2.048 (3)	C5—C6	1.511 (5)
Cr2—N7	2.070 (3)	C5—H5B	0.9700
Cr2—N8	2.091 (3)	C5—H5C	0.9700
Cr2—N6	2.093 (3)	C11—C10	1.511 (6)
O8—C15	1.288 (4)	C11—H11A	0.9700
O4—C7	1.289 (4)	C11—H11B	0.9700
O1—C8	1.299 (4)	C1—C2	1.500 (5)
O3—C7	1.230 (4)	C1—H1B	0.9700
N4—C6	1.475 (4)	C1—H1C	0.9700
N4—H4A	0.9000	C9—C10	1.524 (5)
N4—H4D	0.9000	C9—H9A	0.9700

O6—C16	1.224 (4)	C9—H9B	0.9700
O2—C8	1.213 (4)	C12—C13	1.521 (5)
O5—C16	1.274 (5)	C12—H12A	0.9700
C7—C8	1.554 (5)	C12—H12B	0.9700
N7—C14	1.484 (6)	C6—H6B	0.9700
N7—H7A	0.9000	C6—H6C	0.9700
N7—H7B	0.9000	C2—C3	1.518 (5)
N1—C1	1.483 (4)	C2—H2B	0.9700
N1—H1A	0.9000	C2—H2C	0.9700
N1—H1D	0.9000	C3—H3B	0.9700
N5—C9	1.484 (5)	C3—H3C	0.9700
N5—H5A	0.9000	C10—H10A	0.9700
N5—H5D	0.9000	C10—H10B	0.9700
N8—C12	1.476 (5)	C14—C13	1.503 (5)
N8—H8A	0.9000	C14—H14A	0.9700
N8—H8B	0.9000	C14—H14B	0.9700
C16—C15	1.550 (5)	C13—H13A	0.9700
N3—C4	1.475 (4)	C13—H13B	0.9700
N3—H3A	0.9000	O2W—H200	0.8498
N3—H3D	0.9000	O2W—H201	0.8506
O7—C15	1.234 (4)	O1W—H100	0.8500
N6—C11	1.481 (5)	O1W—H101	0.8500
O4—Cr1—O1	82.29 (9)	Cr1—N2—H2A	107.9
O4—Cr1—N4	88.73 (10)	C3—N2—H2D	107.9
O1—Cr1—N4	170.97 (10)	Cr1—N2—H2D	107.9
O4—Cr1—N2	92.45 (10)	H2A—N2—H2D	107.2
O1—Cr1—N2	91.44 (10)	N3—C4—C5	112.4 (3)
N4—Cr1—N2	89.91 (11)	N3—C4—H4B	109.1
O4—Cr1—N3	90.12 (10)	C5—C4—H4B	109.1
O1—Cr1—N3	87.51 (10)	N3—C4—H4C	109.1
N4—Cr1—N3	91.54 (11)	C5—C4—H4C	109.1
N2—Cr1—N3	177.08 (11)	H4B—C4—H4C	107.9
O4—Cr1—N1	178.36 (11)	C6—C5—C4	113.7 (3)
O1—Cr1—N1	96.87 (10)	C6—C5—H5B	108.8
N4—Cr1—N1	92.13 (11)	C4—C5—H5B	108.8
N2—Cr1—N1	86.15 (10)	C6—C5—H5C	108.8
N3—Cr1—N1	91.26 (10)	C4—C5—H5C	108.8
O5—Cr2—O8	82.47 (10)	H5B—C5—H5C	107.7
O5—Cr2—N5	88.59 (11)	O2—C8—O1	126.1 (3)
O8—Cr2—N5	170.49 (11)	O2—C8—C7	120.8 (3)
O5—Cr2—N7	176.91 (14)	O1—C8—C7	113.1 (3)
O8—Cr2—N7	95.09 (12)	N6—C11—C10	111.5 (3)
N5—Cr2—N7	93.95 (13)	N6—C11—H11A	109.3
O5—Cr2—N8	89.44 (11)	C10—C11—H11A	109.3
O8—Cr2—N8	89.79 (11)	N6—C11—H11B	109.3
N5—Cr2—N8	93.36 (11)	C10—C11—H11B	109.3
N7—Cr2—N8	88.65 (11)	H11A—C11—H11B	108.0
O5—Cr2—N6	91.39 (11)	N1—C1—C2	111.4 (3)
O8—Cr2—N6	89.94 (11)	N1—C1—H1B	109.3

N5—Cr2—N6	87.05 (11)	C2—C1—H1B	109.3
N7—Cr2—N6	90.50 (11)	N1—C1—H1C	109.3
N8—Cr2—N6	179.09 (12)	C2—C1—H1C	109.3
C15—O8—Cr2	113.5 (2)	H1B—C1—H1C	108.0
C7—O4—Cr1	115.4 (2)	N5—C9—C10	112.8 (3)
C8—O1—Cr1	114.7 (2)	N5—C9—H9A	109.0
C6—N4—Cr1	119.1 (2)	C10—C9—H9A	109.0
C6—N4—H4A	107.5	N5—C9—H9B	109.0
Cr1—N4—H4A	107.5	C10—C9—H9B	109.0
C6—N4—H4D	107.5	H9A—C9—H9B	107.8
Cr1—N4—H4D	107.5	N8—C12—C13	112.3 (3)
H4A—N4—H4D	107.0	N8—C12—H12A	109.2
C16—O5—Cr2	114.9 (2)	C13—C12—H12A	109.2
O3—C7—O4	124.5 (3)	N8—C12—H12B	109.2
O3—C7—C8	121.1 (3)	C13—C12—H12B	109.2
O4—C7—C8	114.4 (3)	H12A—C12—H12B	107.9
C14—N7—Cr2	117.2 (2)	N4—C6—C5	113.0 (3)
C14—N7—H7A	108.0	N4—C6—H6B	109.0
Cr2—N7—H7A	108.0	C5—C6—H6B	109.0
C14—N7—H7B	108.0	N4—C6—H6C	109.0
Cr2—N7—H7B	108.0	C5—C6—H6C	109.0
H7A—N7—H7B	107.2	H6B—C6—H6C	107.8
C1—N1—Cr1	115.4 (2)	C1—C2—C3	114.6 (3)
C1—N1—H1A	108.4	C1—C2—H2B	108.6
Cr1—N1—H1A	108.4	C3—C2—H2B	108.6
C1—N1—H1D	108.4	C1—C2—H2C	108.6
Cr1—N1—H1D	108.4	C3—C2—H2C	108.6
H1A—N1—H1D	107.5	H2B—C2—H2C	107.6
C9—N5—Cr2	118.3 (2)	N2—C3—C2	112.5 (3)
C9—N5—H5A	107.7	N2—C3—H3B	109.1
Cr2—N5—H5A	107.7	C2—C3—H3B	109.1
C9—N5—H5D	107.7	N2—C3—H3C	109.1
Cr2—N5—H5D	107.7	C2—C3—H3C	109.1
H5A—N5—H5D	107.1	H3B—C3—H3C	107.8
C12—N8—Cr2	118.9 (2)	C11—C10—C9	114.5 (3)
C12—N8—H8A	107.6	C11—C10—H10A	108.6
Cr2—N8—H8A	107.6	C9—C10—H10A	108.6
C12—N8—H8B	107.6	C11—C10—H10B	108.6
Cr2—N8—H8B	107.6	C9—C10—H10B	108.6
H8A—N8—H8B	107.0	H10A—C10—H10B	107.6
O6—C16—O5	125.1 (4)	N7—C14—C13	111.8 (3)
O6—C16—C15	120.4 (3)	N7—C14—H14A	109.3
O5—C16—C15	114.4 (3)	C13—C14—H14A	109.3
C4—N3—Cr1	117.36 (19)	N7—C14—H14B	109.3
C4—N3—H3A	108.0	C13—C14—H14B	109.3
Cr1—N3—H3A	108.0	H14A—C14—H14B	107.9
C4—N3—H3D	108.0	O7—C15—O8	124.5 (4)
Cr1—N3—H3D	108.0	O7—C15—C16	121.3 (3)
H3A—N3—H3D	107.2	O8—C15—C16	114.2 (3)

C11—N6—Cr2	117.4 (2)	C14—C13—C12	114.3 (3)
C11—N6—H6A	108.0	C14—C13—H13A	108.7
Cr2—N6—H6A	108.0	C12—C13—H13A	108.7
C11—N6—H6D	108.0	C14—C13—H13B	108.7
Cr2—N6—H6D	108.0	C12—C13—H13B	108.7
H6A—N6—H6D	107.2	H13A—C13—H13B	107.6
C3—N2—Cr1	117.5 (2)	H200—O2W—H201	106.9
C3—N2—H2A	107.9	H100—O1W—H101	111.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4A···Cl2^{i}	0.90	2.46	3.353 (4)	172
N4—H4D···O3^{ii}	0.90	2.02	2.913 (4)	175
N7—H7A···O7^{iii}	0.90	2.12	2.994 (5)	164
N7—H7B···Cl2	0.90	2.54	3.323 (4)	145
N1—H1A···O7^{iv}	0.90	2.16	3.047 (4)	170
N1—H1D···O3^{ii}	0.90	2.39	3.141 (5)	141
N5—H5A···O6^{iii}	0.90	1.97	2.780 (4)	149
N5—H5D···Cl1	0.90	2.28	3.160 (4)	165
N8—H8A···Cl2^{v}	0.90	2.50	3.329 (3)	154
N8—H8B···Cl1	0.90	2.69	3.383 (4)	135
N3—H3A···O7^{iv}	0.90	2.23	3.064 (4)	155
N3—H3D···O2W	0.90	2.15	3.000 (4)	157
N6—H6A···O1^{vi}	0.90	2.47	3.248 (4)	145
N6—H6D···Cl2	0.90	2.47	3.360 (3)	171
N2—H2A···O2^{ii}	0.90	2.53	3.363 (4)	154
N2—H2D···Cl1^{vii}	0.90	2.56	3.323 (3)	143
O1W—H100···Cl1	0.85	2.47	3.169 (4)	140
O1W—H101···O5	0.85	2.29	3.082 (5)	154
O2W—H200···Cl2^{iv}	0.85	2.49	3.298 (4)	160
O2W—H201···O1W^{iii}	0.85	1.95	2.800 (4)	173

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

Fig. 1

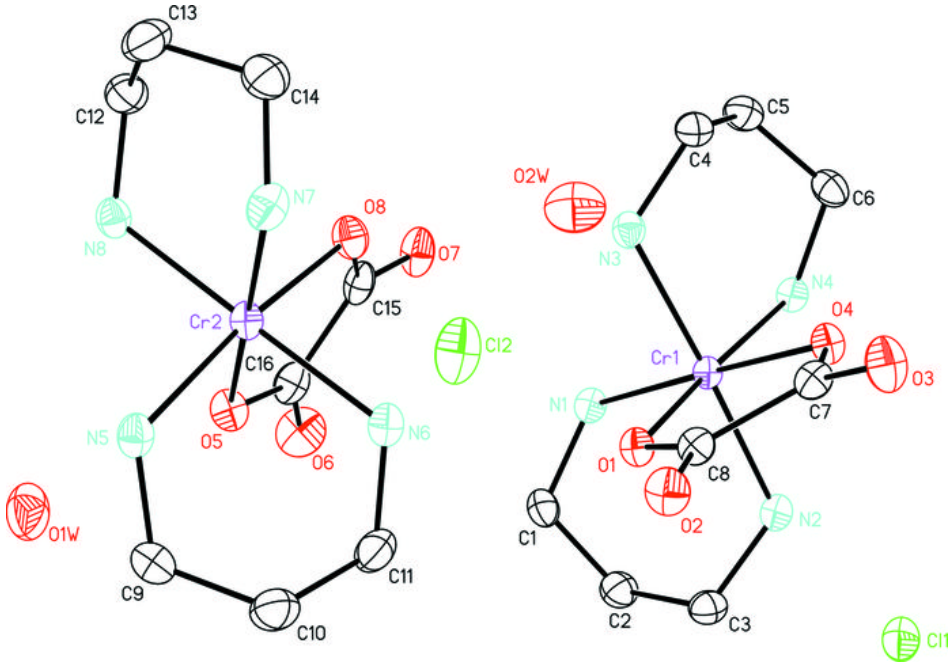
C13
C14
C12
N7
O8
O7
N8
C15
Cr2
Cl2
C16
N5
O5
O6
N6
O1W
C9
C11
C10
C5
C4
O2W
C6
N3
N4
O4
Cr1
O3
N1
C7
O1
C8
O2
N2
C1
C2
C3
Cl1

Fig. 2