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Bis{*N*-[2-(2-hydroxyethylamino)ethyl]-salicylideneiminato-κ^3O,N,N'}-chromium(III) chloride

Yu-Zhou Yuan, Jian Zhou* and Xing Liu

Department of Chemistry and Biology, Yulin Normal University, Yulin 537000, People's Republic of China
Correspondence e-mail: jianzhou888888@163.com

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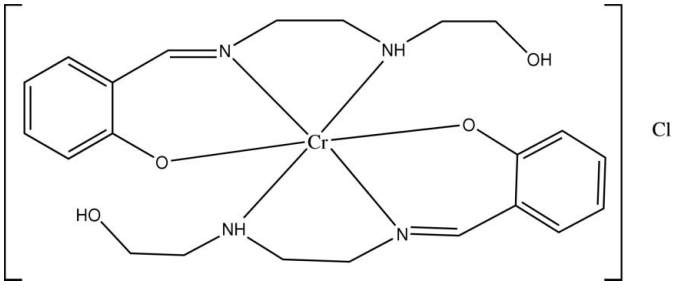
Key indicators: single-crystal X-ray study; T = 153 K; mean σ(C–C) = 0.004 Å; R factor = 0.038; wR factor = 0.149; data-to-parameter ratio = 16.9.

In the title complex, $[Cr(C_{11}H_{15}N_2O_2)_2]Cl$, the Cr^{III} ion is coordinated by four N atoms and two O atoms from two tridentate *N*-[2-(2-hydroxyethylamino)ethyl]salicylideneimine (sadol) ligands to form a distorted octahedron. A centrosymmetric dimer is constructed through the formation of O—H···Cl and N—H···Cl hydrogen bonds.

Related literature

For related literature, see: Choi *et al.* (2003); Cornman *et al.* (1992); Cros *et al.* (1987); Darensbourg *et al.* (2004); Gabriel *et al.* (2007); Haber *et al.* (2003); Li *et al.* (1988); Plass (1996); Qiu *et al.* (2004); Taylor (1978); Usman *et al.* (2003); Vaqueiro *et al.* (2003); Yang *et al.* (2004); Zhu, Lin, Meng, Zou & Wang (2003); Zhu, Liu, Wang & Wang (2003).



Experimental

Crystal data

$[Cr(C_{11}H_{15}N_2O_2)_2]Cl$
M_r = 501.95
Monoclinic, $P2_1/n$
a = 9.8883 (3) Å
b = 24.6255 (6) Å
c = 10.3494 (4) Å
β = 116.3880 (10)°
V = 2257.54 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.66 mm^{-1}
T = 153 (2) K
0.15 × 0.13 × 0.09 mm

Data collection

Rigaku R-AXIS Spider diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.907, T_{max} = 0.945
21950 measured reflections
5165 independent reflections
4097 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.149
S = 1.06
5165 reflections
306 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*O*···Cl1	0.86 (5)	2.31 (5)	3.175 (3)	178 (4)
O4—H4*O*···Cl1^{i}	0.78 (4)	2.54 (4)	3.229 (3)	149 (4)
N4—H4*N*···Cl1	0.85 (4)	2.62 (4)	3.457 (3)	168 (4)
N2—H2*N*···Cl1	0.87 (3)	2.30 (3)	3.170 (2)	177 (3)

Symmetry code: (i) $-x, -y+1, -z$.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1995); 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: FJ2018).

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supplementary materials

Acta Cryst. (2007). E**63**, m1580-m1581 [**doi:10.1107/S1600536807021289**]

Bis{*N*-[2-(2-hydroxyethylamino)ethyl]salicylideneiminato-κ^3O,N,N'}chromium(III) chloride

Y.-Z. Yuan, J. Zhou and X. Liu

Comment

During the past decades, complexes of *N*-(2-(2-hydroxyethylamino)ethyl) salicylideneimine Schiff base (sadol) and its derivatives with transition metal have attracted considerable interest because of their potential applications in biological and magnetic properties (Plass, 1996; Cros *et al.*, 1987; Li *et al.*, 1988). Some structurally related complexes of sadol have been reported. These examples include mono-nuclear structures, such as $Cd(sadol)_2.2H_2O$ (Yang *et al.*, 2004), [VO(sadol)(acac)] (Li *et al.*, 1988), VO(sadol)(cat) (Cornman *et al.*, 1992), $[ZnCl_2(sadol)]$ (Usman *et al.*, 2003) and $[Co(sadol)_2]Cl$ (Zhu, *et al.*, 2003), and dimers, as exemplified by $[VO_2(sadol)]_2$ (Li *et al.*, 1988), $[\{Cd(sadol)(ClO_4)\}_2]$ (Haber *et al.*, 2003) and $[\{Zn(sadol)\}_2SO_4]$ (Qiu *et al.*, 2004). As an extension of these studies, we report here the structure of $[Cr(C_{11}H_{15}N_2O_2)_2]Cl$, (I).

The complex consists of discrete $[Cr(sadol)_2]^+$ cations with chloride anions as counterions (Fig. 1, Table 1). The Cr(III) ion is coordinated by four N atoms and two phenoxo O atoms from two sadol ligands to form a slightly distorted octahedron, which can be seen from the *trans*-angles varying from 172.00 (9) to 172.26 (8) ° and the *cis*-angles in the range of 81.76 (9)–95.25 (9)°, respectively. Chelation of Cr by the sadol ligand forms a six-membered ring and a five-membered ring, which contribute to the stability of the complex cation. The hydroxy O atom is non-coordinating, mainly because the coordination sphere of the metal ion is completed by two tri-dentate sadol ligands. This phenomenon is observed in $Cd(sadol)_2{\cdot}2H_2O$ (Yang *et al.*, 2004) and $Co(sadol)_2{\cdot}NO_3$ (Zhu, *et al.*, 2003). The Cr—O bond distances are 1.9207 (19) Å for Cr1—O1 and 1.929 (2) Å for Cr1—O3 and are shorter than those in other Cr(III) oxygen-containing complexes, $(NH_4)_4[Cr(C_6H_4O_7)(C_6H_5O_7)]{\cdot}3H_2O$ [1.933 (2)–1.993 (2) Å] (Gabriel *et al.*, 2007), $K_3[Cr(C_2O_4)_3]{\cdot}3H_2O$ [1.955 (2)–1.985 (2) Å] (Taylor, 1978) and $K_2[Cr_2(C_6H_6NO_6)_2(OH)_2]{\cdot}6H_2O$ [1.937 (4)–1.983 (3) Å] (Choi, 2003). The Cr—N bond lengths ranging from 2.009 (2) to 2.135 (2) Å are in agreement with corresponding bond distances in $[Cr(C_6H_{18}N_4)(SbS_3)]$ (Vaqueiro *et al.*, 2003) and (salen)Cr(III)*X* (*X*=Cl, N_3) (Darensbourg *et al.*, 2004).

In I, two $[Cr(sadol)_2]^+$ cations are linked into a centro-symmetric dimer by four O—H···Cl and two N—H···Cl hydrogen bonds, all involving the Cl anion as the acceptor (Fig. 2).

Experimental

Single crystals of the title complex suitable for X-ray crystallographic analysis were obtained by solvothermal treatment of $CrCl_3{\cdot}6H_2O$ (0.2 mmol) and salicylaldehyde (0.4 mmol),2-hydroxyaminoethylamine (0.4 mmol) and ethanol (3 ml). The reagents were placed in a thick Pyrex tube (*ca* 20 cm long). The tube was cooled with liquid N_2 and the air evacuated. The sealed tube was heated at 353 K for 4 d to yield brown chunk crystals in about 43% yield.

Refinement

H atoms on the C atoms were positioned geometrically and were allowed to ride on their parent atoms, with C—H = 0.95 Å or 0.99 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C). H atoms on the O and N atoms were located from difference Fourier maps and freely refined.

Figures

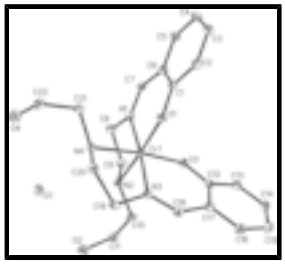

Fig. 1. The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level, and all H atoms are omitted for clarity.

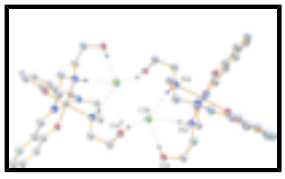

Fig. 2. The centrosymmetric dimer constructed by the combination of O—H···Cl and N—H···Cl hydrogen bonds. [Symmetry code: (i) −*x*, −*y* + 1, −*z*.]

Bis{*N*-[2-(2-hydroxyethylamino)ethyl]salicylideneimine-κ^3*O*,*N*,*N*'} chromium(III) chloride

Crystal data

$[Cr(C_{11}H_{15}N_2O_2)_2]Cl$	F_{000} = 1052
M_r = 501.95	D_x = 1.477 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 22244 reflections
a = 9.8883 (3) Å	θ = 3.3–27.5º
b = 24.6255 (6) Å	μ = 0.66 mm^{-1}
c = 10.3494 (4) Å	T = 153 (2) K
β = 116.3880 (10)º	Block, brown
V = 2257.54 (12) Å^3	0.15 × 0.13 × 0.09 mm
Z = 4	

Data collection

Rigaku R-AXIS Spider diffractometer	5165 independent reflections
Radiation source: Rotating anode	4097 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.047
T = 153(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.3º

Absorption correction: empirical (using intensity measurements) (ABSCOR; Higashi, 1995)	$h = -12 \rightarrow 12$
$T_{min} = 0.907$, $T_{max} = 0.945$	$k = -31 \rightarrow 31$
21950 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
$R[F^2 > 2\sigma(F^2)] = 0.038$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.149$	$w = 1/[\sigma^2(F_o^2) + (0.0798P)^2 + 2.5978P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
5165 reflections	$\Delta\rho_{max} = 0.59$ e Å^{-3}
306 parameters	$\Delta\rho_{min} = -0.77$ 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	0.25588 (5)	0.639340 (16)	0.37527 (5)	0.01611 (15)
Cl1	−0.00302 (9)	0.49037 (3)	0.19134 (9)	0.0312 (2)
O1	0.4222 (2)	0.67803 (7)	0.3704 (2)	0.0216 (4)
O2	−0.2439 (3)	0.55214 (9)	0.2622 (3)	0.0319 (5)
O3	0.2469 (2)	0.68784 (7)	0.5176 (2)	0.0204 (4)
O4	0.3031 (3)	0.48259 (9)	0.1011 (3)	0.0351 (6)
N1	0.4013 (3)	0.58897 (9)	0.5279 (3)	0.0192 (5)
N2	0.0960 (3)	0.59080 (9)	0.4053 (3)	0.0189 (5)
N3	0.1005 (3)	0.68405 (9)	0.2162 (3)	0.0191 (5)
N4	0.2410 (3)	0.59186 (9)	0.1968 (3)	0.0195 (5)
C1	0.5654 (3)	0.67774 (10)	0.4665 (3)	0.0190 (5)
C2	0.6616 (3)	0.71784 (11)	0.4563 (3)	0.0235 (6)

H2A	0.6216	0.7442	0.3816	0.028*
C3	0.8124 (3)	0.71979 (12)	0.5522 (4)	0.0291 (7)
H3A	0.8744	0.7476	0.5435	0.035*
C4	0.8749 (3)	0.68135 (13)	0.6616 (4)	0.0298 (7)
H4A	0.9793	0.6826	0.7269	0.036*
C5	0.7842 (3)	0.64169 (12)	0.6740 (3)	0.0267 (6)
H5A	0.8270	0.6154	0.7484	0.032*
C6	0.6293 (3)	0.63902 (11)	0.5792 (3)	0.0204 (6)
C7	0.5446 (3)	0.59572 (11)	0.6021 (3)	0.0211 (6)
H7A	0.5979	0.5704	0.6770	0.025*
C8	0.3264 (3)	0.54421 (11)	0.5645 (3)	0.0257 (6)
H8A	0.3898	0.5315	0.6641	0.031*
H8B	0.3087	0.5134	0.4975	0.031*
C9	0.1781 (3)	0.56623 (11)	0.5511 (3)	0.0246 (6)
H9A	0.1173	0.5366	0.5637	0.029*
H9B	0.1965	0.5940	0.6263	0.029*
C10	−0.0439 (3)	0.61895 (11)	0.3877 (3)	0.0241 (6)
H10A	−0.0862	0.6387	0.2948	0.029*
H10B	−0.0168	0.6463	0.4655	0.029*
C11	−0.1655 (3)	0.58246 (11)	0.3909 (3)	0.0251 (6)
H11A	−0.1188	0.5569	0.4729	0.030*
H11B	−0.2390	0.6050	0.4078	0.030*
C12	0.1824 (3)	0.73617 (10)	0.4983 (3)	0.0202 (6)
C13	0.1971 (3)	0.76508 (11)	0.6207 (3)	0.0235 (6)
H13A	0.2506	0.7491	0.7133	0.028*
C14	0.1356 (3)	0.81617 (12)	0.6095 (4)	0.0267 (6)
H14A	0.1479	0.8349	0.6943	0.032*
C15	0.0555 (4)	0.84056 (12)	0.4752 (4)	0.0296 (7)
H15A	0.0158	0.8762	0.4680	0.035*
C16	0.0350 (3)	0.81254 (11)	0.3542 (4)	0.0266 (6)
H16A	−0.0224	0.8285	0.2622	0.032*
C17	0.0974 (3)	0.76009 (10)	0.3626 (3)	0.0202 (6)
C18	0.0578 (3)	0.73256 (10)	0.2282 (3)	0.0195 (5)
H18A	−0.0044	0.7514	0.1419	0.023*
C19	0.0393 (3)	0.65791 (11)	0.0744 (3)	0.0221 (6)
H19A	−0.0012	0.6856	−0.0028	0.027*
H19B	−0.0436	0.6329	0.0630	0.027*
C20	0.1661 (3)	0.62671 (11)	0.0640 (3)	0.0224 (6)
H20A	0.1254	0.6037	−0.0235	0.027*
H20B	0.2403	0.6523	0.0578	0.027*
C21	0.3885 (3)	0.57035 (12)	0.2107 (3)	0.0258 (6)
H21A	0.4408	0.5517	0.3049	0.031*
H21B	0.4523	0.6014	0.2109	0.031*
C22	0.3754 (3)	0.53118 (12)	0.0926 (3)	0.0274 (6)
H22A	0.3167	0.5483	−0.0028	0.033*
H22B	0.4773	0.5227	0.1023	0.033*
H2O	−0.180 (5)	0.5348 (18)	0.242 (5)	0.053 (13)*
H4O	0.220 (5)	0.4791 (16)	0.044 (5)	0.038 (12)*
H2N	0.072 (4)	0.5629 (13)	0.347 (4)	0.018 (8)*

H4N	0.187 (4)	0.5638 (15)	0.188 (4)	0.030 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cr1	0.0146 (2)	0.0155 (2)	0.0183 (2)	0.00028 (14)	0.00737 (18)	0.00112 (15)
Cl1	0.0317 (4)	0.0273 (4)	0.0337 (4)	−0.0050 (3)	0.0138 (3)	−0.0070 (3)
O1	0.0149 (9)	0.0214 (9)	0.0269 (10)	−0.0021 (7)	0.0077 (8)	0.0030 (8)
O2	0.0215 (11)	0.0381 (12)	0.0356 (13)	−0.0032 (9)	0.0122 (10)	−0.0023 (10)
O3	0.0223 (10)	0.0183 (9)	0.0196 (9)	0.0023 (7)	0.0085 (8)	0.0011 (7)
O4	0.0370 (14)	0.0282 (11)	0.0336 (13)	0.0027 (10)	0.0099 (11)	0.0004 (10)
N1	0.0181 (11)	0.0179 (10)	0.0231 (12)	0.0024 (8)	0.0104 (9)	0.0018 (9)
N2	0.0174 (11)	0.0175 (10)	0.0234 (12)	0.0004 (8)	0.0106 (9)	0.0010 (9)
N3	0.0164 (11)	0.0207 (10)	0.0202 (11)	−0.0006 (8)	0.0081 (9)	0.0007 (9)
N4	0.0183 (11)	0.0182 (10)	0.0222 (12)	−0.0005 (9)	0.0089 (9)	−0.0016 (9)
C1	0.0156 (12)	0.0204 (12)	0.0237 (14)	0.0000 (9)	0.0113 (11)	−0.0038 (10)
C2	0.0229 (14)	0.0213 (12)	0.0298 (15)	−0.0022 (10)	0.0150 (12)	−0.0013 (11)
C3	0.0256 (15)	0.0279 (14)	0.0383 (17)	−0.0078 (12)	0.0182 (14)	−0.0097 (13)
C4	0.0183 (14)	0.0370 (16)	0.0307 (16)	−0.0056 (12)	0.0077 (12)	−0.0071 (13)
C5	0.0225 (14)	0.0328 (15)	0.0234 (14)	0.0014 (12)	0.0089 (12)	−0.0002 (12)
C6	0.0215 (14)	0.0246 (13)	0.0160 (13)	−0.0006 (10)	0.0090 (11)	−0.0027 (10)
C7	0.0196 (13)	0.0208 (12)	0.0220 (13)	0.0042 (10)	0.0085 (11)	0.0014 (10)
C8	0.0207 (14)	0.0212 (13)	0.0339 (16)	0.0017 (10)	0.0109 (12)	0.0119 (12)
C9	0.0249 (14)	0.0246 (13)	0.0261 (15)	−0.0001 (11)	0.0130 (12)	0.0085 (11)
C10	0.0190 (13)	0.0212 (12)	0.0351 (16)	0.0028 (10)	0.0148 (12)	0.0055 (12)
C11	0.0221 (14)	0.0248 (13)	0.0327 (16)	0.0025 (11)	0.0161 (12)	0.0069 (12)
C12	0.0150 (12)	0.0186 (12)	0.0281 (15)	−0.0030 (10)	0.0107 (11)	−0.0010 (10)
C13	0.0197 (13)	0.0265 (13)	0.0237 (14)	−0.0016 (11)	0.0091 (11)	−0.0030 (11)
C14	0.0236 (14)	0.0274 (14)	0.0315 (16)	−0.0032 (11)	0.0144 (13)	−0.0087 (12)
C15	0.0322 (16)	0.0198 (13)	0.0373 (17)	0.0030 (12)	0.0160 (14)	−0.0022 (12)
C16	0.0274 (15)	0.0204 (13)	0.0336 (16)	0.0026 (11)	0.0149 (13)	0.0037 (12)
C17	0.0196 (13)	0.0170 (12)	0.0274 (14)	−0.0002 (10)	0.0134 (11)	0.0020 (10)
C18	0.0182 (12)	0.0206 (12)	0.0226 (13)	0.0001 (10)	0.0117 (11)	0.0039 (10)
C19	0.0200 (13)	0.0244 (13)	0.0163 (13)	0.0025 (11)	0.0030 (11)	0.0005 (11)
C20	0.0271 (14)	0.0256 (13)	0.0143 (12)	0.0020 (11)	0.0090 (11)	−0.0017 (11)
C21	0.0189 (13)	0.0301 (14)	0.0272 (15)	0.0030 (11)	0.0092 (12)	−0.0047 (12)
C22	0.0257 (15)	0.0317 (15)	0.0261 (15)	0.0041 (12)	0.0128 (13)	−0.0033 (12)

Geometric parameters (Å, °)

Cr1—O1	1.9207 (19)	C7—H7A	0.9500
Cr1—O3	1.929 (2)	C8—C9	1.512 (4)
Cr1—N3	2.009 (2)	C8—H8A	0.9900
Cr1—N1	2.020 (2)	C8—H8B	0.9900
Cr1—N2	2.112 (2)	C9—H9A	0.9900
Cr1—N4	2.135 (2)	C9—H9B	0.9900
O1—C1	1.321 (3)	C10—C11	1.513 (4)
O2—C11	1.419 (4)	C10—H10A	0.9900
O2—H2O	0.86 (5)	C10—H10B	0.9900

O3—C12	1.323 (3)	C11—H11A	0.9900
O4—C22	1.417 (4)	C11—H11B	0.9900
O4—H4O	0.78 (4)	C12—C13	1.404 (4)
N1—C7	1.288 (4)	C12—C17	1.406 (4)
N1—C8	1.468 (3)	C13—C14	1.380 (4)
N2—C10	1.485 (3)	C13—H13A	0.9500
N2—C9	1.488 (4)	C14—C15	1.394 (5)
N2—H2N	0.87 (3)	C14—H14A	0.9500
N3—C18	1.292 (3)	C15—C16	1.364 (4)
N3—C19	1.465 (3)	C15—H15A	0.9500
N4—C21	1.497 (4)	C16—C17	1.417 (4)
N4—C20	1.506 (3)	C16—H16A	0.9500
N4—H4N	0.85 (4)	C17—C18	1.436 (4)
C1—C2	1.407 (4)	C18—H18A	0.9500
C1—C6	1.419 (4)	C19—C20	1.514 (4)
C2—C3	1.377 (4)	C19—H19A	0.9900
C2—H2A	0.9500	C19—H19B	0.9900
C3—C4	1.392 (5)	C20—H20A	0.9900
C3—H3A	0.9500	C20—H20B	0.9900
C4—C5	1.370 (4)	C21—C22	1.517 (4)
C4—H4A	0.9500	C21—H21A	0.9900
C5—C6	1.406 (4)	C21—H21B	0.9900
C5—H5A	0.9500	C22—H22A	0.9900
C6—C7	1.439 (4)	C22—H22B	0.9900
O1—Cr1—O3	92.51 (9)	N2—C9—C8	107.9 (2)
O1—Cr1—N3	93.34 (9)	N2—C9—H9A	110.1
O3—Cr1—N3	90.50 (9)	C8—C9—H9A	110.1
O1—Cr1—N1	90.29 (9)	N2—C9—H9B	110.1
O3—Cr1—N1	92.37 (9)	C8—C9—H9B	110.1
N3—Cr1—N1	175.27 (9)	H9A—C9—H9B	108.4
O1—Cr1—N2	172.00 (9)	N2—C10—C11	115.2 (2)
O3—Cr1—N2	86.94 (9)	N2—C10—H10A	108.5
N3—Cr1—N2	94.65 (9)	C11—C10—H10A	108.5
N1—Cr1—N2	81.76 (9)	N2—C10—H10B	108.5
O1—Cr1—N4	88.80 (9)	C11—C10—H10B	108.5
O3—Cr1—N4	172.26 (8)	H10A—C10—H10B	107.5
N3—Cr1—N4	81.80 (9)	O2—C11—C10	113.6 (3)
N1—Cr1—N4	95.25 (9)	O2—C11—H11A	108.9
N2—Cr1—N4	92.81 (9)	C10—C11—H11A	108.9
C1—O1—Cr1	128.43 (18)	O2—C11—H11B	108.9
C11—O2—H2O	109 (3)	C10—C11—H11B	108.9
C12—O3—Cr1	128.60 (18)	H11A—C11—H11B	107.7
C22—O4—H4O	116 (3)	O3—C12—C13	118.0 (3)
C7—N1—C8	119.3 (2)	O3—C12—C17	124.2 (3)
C7—N1—Cr1	126.83 (19)	C13—C12—C17	117.7 (2)
C8—N1—Cr1	113.43 (17)	C14—C13—C12	121.5 (3)
C10—N2—C9	111.8 (2)	C14—C13—H13A	119.3
C10—N2—Cr1	115.81 (16)	C12—C13—H13A	119.3
C9—N2—Cr1	105.84 (17)	C13—C14—C15	120.7 (3)

C10—N2—H2N	109 (2)	C13—C14—H14A	119.7
C9—N2—H2N	104 (2)	C15—C14—H14A	119.7
Cr1—N2—H2N	110 (2)	C16—C15—C14	119.0 (3)
C18—N3—C19	119.7 (2)	C16—C15—H15A	120.5
C18—N3—Cr1	126.3 (2)	C14—C15—H15A	120.5
C19—N3—Cr1	113.92 (17)	C15—C16—C17	121.4 (3)
C21—N4—C20	110.7 (2)	C15—C16—H16A	119.3
C21—N4—Cr1	114.89 (17)	C17—C16—H16A	119.3
C20—N4—Cr1	107.10 (16)	C12—C17—C16	119.6 (3)
C21—N4—H4N	105 (2)	C12—C17—C18	123.6 (2)
C20—N4—H4N	109 (3)	C16—C17—C18	116.6 (3)
Cr1—N4—H4N	110 (3)	N3—C18—C17	124.8 (3)
O1—C1—C2	118.3 (2)	N3—C18—H18A	117.6
O1—C1—C6	124.0 (2)	C17—C18—H18A	117.6
C2—C1—C6	117.7 (3)	N3—C19—C20	107.9 (2)
C3—C2—C1	121.5 (3)	N3—C19—H19A	110.1
C3—C2—H2A	119.3	C20—C19—H19A	110.1
C1—C2—H2A	119.3	N3—C19—H19B	110.1
C2—C3—C4	120.6 (3)	C20—C19—H19B	110.1
C2—C3—H3A	119.7	H19A—C19—H19B	108.4
C4—C3—H3A	119.7	N4—C20—C19	108.2 (2)
C5—C4—C3	119.2 (3)	N4—C20—H20A	110.1
C5—C4—H4A	120.4	C19—C20—H20A	110.1
C3—C4—H4A	120.4	N4—C20—H20B	110.1
C4—C5—C6	121.6 (3)	C19—C20—H20B	110.1
C4—C5—H5A	119.2	H20A—C20—H20B	108.4
C6—C5—H5A	119.2	N4—C21—C22	114.6 (2)
C5—C6—C1	119.4 (3)	N4—C21—H21A	108.6
C5—C6—C7	116.9 (3)	C22—C21—H21A	108.6
C1—C6—C7	123.7 (3)	N4—C21—H21B	108.6
N1—C7—C6	124.3 (3)	C22—C21—H21B	108.6
N1—C7—H7A	117.8	H21A—C21—H21B	107.6
C6—C7—H7A	117.8	O4—C22—C21	110.6 (3)
N1—C8—C9	106.7 (2)	O4—C22—H22A	109.5
N1—C8—H8A	110.4	C21—C22—H22A	109.5
C9—C8—H8A	110.4	O4—C22—H22B	109.5
N1—C8—H8B	110.4	C21—C22—H22B	109.5
C9—C8—H8B	110.4	H22A—C22—H22B	108.1
H8A—C8—H8B	108.6		
O3—Cr1—O1—C1	75.1 (2)	C2—C3—C4—C5	−0.7 (5)
N3—Cr1—O1—C1	165.7 (2)	C3—C4—C5—C6	−0.3 (5)
N1—Cr1—O1—C1	−17.3 (2)	C4—C5—C6—C1	1.0 (4)
N4—Cr1—O1—C1	−112.5 (2)	C4—C5—C6—C7	−179.9 (3)
O1—Cr1—O3—C12	81.4 (2)	O1—C1—C6—C5	178.5 (3)
N3—Cr1—O3—C12	−12.0 (2)	C2—C1—C6—C5	−0.8 (4)
N1—Cr1—O3—C12	171.8 (2)	O1—C1—C6—C7	−0.4 (4)
N2—Cr1—O3—C12	−106.6 (2)	C2—C1—C6—C7	−179.7 (3)
O1—Cr1—N1—C7	13.2 (2)	C8—N1—C7—C6	−178.0 (3)
O3—Cr1—N1—C7	−79.3 (2)	Cr1—N1—C7—C6	−5.9 (4)

N2—Cr1—N1—C7	−165.8 (3)	C5—C6—C7—N1	177.5 (3)
N4—Cr1—N1—C7	102.1 (2)	C1—C6—C7—N1	−3.5 (4)
O1—Cr1—N1—C8	−174.3 (2)	C7—N1—C8—C9	139.3 (3)
O3—Cr1—N1—C8	93.2 (2)	Cr1—N1—C8—C9	−33.8 (3)
N2—Cr1—N1—C8	6.7 (2)	C10—N2—C9—C8	−173.7 (2)
N4—Cr1—N1—C8	−85.4 (2)	Cr1—N2—C9—C8	−46.8 (2)
O3—Cr1—N2—C10	53.9 (2)	N1—C8—C9—N2	53.2 (3)
N3—Cr1—N2—C10	−36.3 (2)	C9—N2—C10—C11	−66.0 (3)
N1—Cr1—N2—C10	146.8 (2)	Cr1—N2—C10—C11	172.7 (2)
N4—Cr1—N2—C10	−118.3 (2)	N2—C10—C11—O2	−75.3 (3)
O3—Cr1—N2—C9	−70.60 (17)	Cr1—O3—C12—C13	−177.08 (19)
N3—Cr1—N2—C9	−160.85 (18)	Cr1—O3—C12—C17	4.3 (4)
N1—Cr1—N2—C9	22.25 (17)	O3—C12—C13—C14	178.8 (3)
N4—Cr1—N2—C9	117.15 (18)	C17—C12—C13—C14	−2.5 (4)
O1—Cr1—N3—C18	−77.8 (2)	C12—C13—C14—C15	0.4 (5)
O3—Cr1—N3—C18	14.7 (2)	C13—C14—C15—C16	1.9 (5)
N2—Cr1—N3—C18	101.7 (2)	C14—C15—C16—C17	−2.1 (5)
N4—Cr1—N3—C18	−166.1 (2)	O3—C12—C17—C16	−179.1 (3)
O1—Cr1—N3—C19	99.16 (19)	C13—C12—C17—C16	2.3 (4)
O3—Cr1—N3—C19	−168.30 (19)	O3—C12—C17—C18	6.4 (4)
N2—Cr1—N3—C19	−81.33 (19)	C13—C12—C17—C18	−172.2 (3)
N4—Cr1—N3—C19	10.85 (19)	C15—C16—C17—C12	0.0 (4)
O1—Cr1—N4—C21	46.7 (2)	C15—C16—C17—C18	174.8 (3)
N3—Cr1—N4—C21	140.2 (2)	C19—N3—C18—C17	173.2 (3)
N1—Cr1—N4—C21	−43.5 (2)	Cr1—N3—C18—C17	−10.0 (4)
N2—Cr1—N4—C21	−125.5 (2)	C12—C17—C18—N3	−3.1 (4)
O1—Cr1—N4—C20	−76.64 (18)	C16—C17—C18—N3	−177.7 (3)
N3—Cr1—N4—C20	16.91 (17)	C18—N3—C19—C20	140.8 (3)
N1—Cr1—N4—C20	−166.82 (18)	Cr1—N3—C19—C20	−36.4 (3)
N2—Cr1—N4—C20	111.20 (18)	C21—N4—C20—C19	−166.5 (2)
Cr1—O1—C1—C2	−166.48 (19)	Cr1—N4—C20—C19	−40.6 (2)
Cr1—O1—C1—C6	14.2 (4)	N3—C19—C20—N4	50.4 (3)
O1—C1—C2—C3	−179.5 (3)	C20—N4—C21—C22	−65.6 (3)
C6—C1—C2—C3	−0.2 (4)	Cr1—N4—C21—C22	173.0 (2)
C1—C2—C3—C4	0.9 (5)	N4—C21—C22—O4	−66.5 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2O···Cl1	0.86 (5)	2.31 (5)	3.175 (3)	178 (4)
O4—H4O···Cl1^{i}	0.78 (4)	2.54 (4)	3.229 (3)	149 (4)
N4—H4N···Cl1	0.85 (4)	2.62 (4)	3.457 (3)	168 (4)
N2—H2N···Cl1	0.87 (3)	2.30 (3)	3.170 (2)	177 (3)

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

Fig. 1

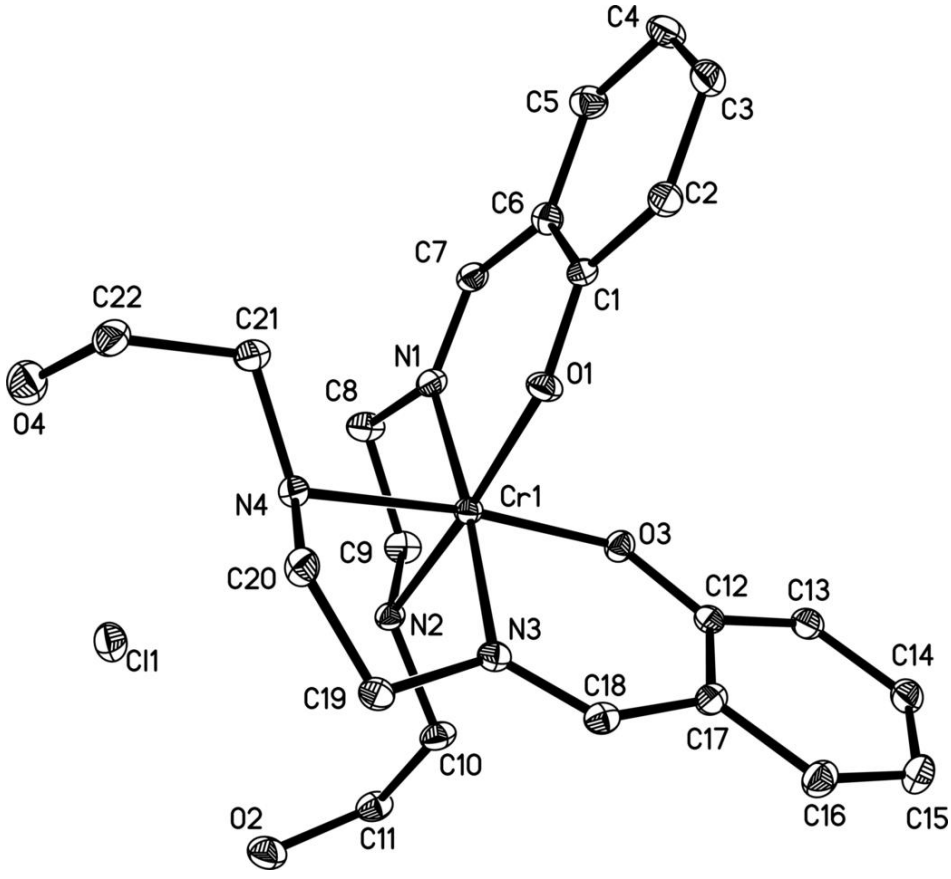
C4
C5
C3
C6
C2
C7
C1
C22
C21
N1
O1
C8
O4
N4
Cr1
O3
C9
C20
C12
C13
N2
N3
Cl1
C14
C19
C18
C17
C10
O2
C11
C16
C15

Fig. 2