Crystal structure of 1,4,8,11-tetramethyl-1,4,8,11-tetraazoniacyclotetradecane bis[chlorido-chromate(VI)] dichloride from synchrotron X-ray data

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The crystal structure of title compound, $(C_{14}H_{36}N_4)[CrO_3Cl]_2Cl_2$, has been determined by synchrotron radiation X-ray crystallography at 220 K. The macrocyclic cation lies across a crystallographic inversion center and hence the asymmetric unit contains one half of the organic cation, one chlorochromate anion and one chloride anion. Both the Cl^- anion and chlorochromate Cl atom are involved in hydrogen bonding. In the crystal, hydrogen bonds involving the 1,4,8,11-tetramethyl-1,4,8,11-tetraazoniacyclotetradecane (TMC) N—H groups and C—H groups as donor groups and three O atoms of the chlorochromate and the chloride anion as acceptor groups link the components, giving rise to a three-dimensional network.

1. Chemical context

Chromium(VI) compounds have a toxic and genotoxic character to humans and wildlife (Yusof & Malek, 2009), but they are very important in industrial processes (Goyal *et al.*, 2003). 1,4,8,11-Tetraazacyclotetradecane and its substituted derivatives are involved in diverse application fields such as catalysis, enzyme mimics, chemical sensors, selective metal-ion recovery, pharmacology and therapy (Meyer *et al.*, 1998). Tetra-*N*-methylated 1,4,8,11-tetramethyl-1,4,8,11-tetraazacyclotetradecane (TMC, $C_{14}H_{36}N_4$) is basic and readily captures protons to form a dication, $C_{14}H_{34}N_4^{2+}$, or tetracation, $C_{14}H_{36}N_4^{4+}$, in which the N—H bonds are generally active in hydrogen-bond formation. These organic cations may be suitable for use in the removal of toxic metal ions.

Previously, the crystal structures of $[H_4TMC](ClO_4)_2Cl_2$ (Moon & Choi, 2020), $[H_2TMC][As_4O_2Cl_{10}]$, $[H_2TMC][Sb_2OCl_6]$ (Willey *et al.*, 1993), $[H_4TMC]_2[Sb_4F_{15}][HF_2]F_4$ (Becker & Mattes, 1996), $[H_4TMC][H_2TMC][W(CN)_8]_2\cdot4H_2O$ (Nowicka *et al.*, 2012) and $[Al(CH_3)_4][TMC]$ (Robinson *et al.*, 1987) were determined, but there is no report of a compound with any combination of the 1,4,8,11-tetramethyl-1,4,8,11-tetraazoniacyclotetradecane cation and CrO_3Cl^- anion. In this communication, we report on the preparation of a new organic chlorochromate $[H_4TMC][CrO_3Cl]_2Cl_2$, (I), and its structural characterization by synchrotron single-crystal X-ray diffraction.
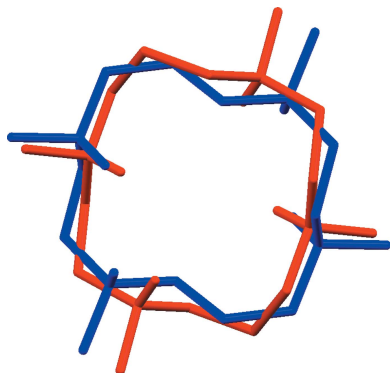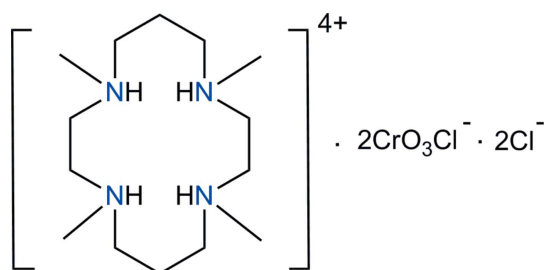
2. Structural commentary

The molecular structure of (I) is shown in Fig. 1 along with the atom-numbering scheme. The organic cation lies across a crystallographic inversion center and hence the asymmetric unit contains one half of the organic cation, one chlorochromate(VI) anion and one chloride anion. The conformation of the tetracation in (I) (blue) is similar to that observed in $[H_4TMC](ClO_4)_2Cl_2$ (red) (Fig. 2; r.m.s. deviation overlay = 0.5878 Å), but it is different from the *trans*-I and *trans*-III conformations of the dications in $[H_2TMC][As_4O_2Cl_{10}]$ and $[H_2TMC][Sb_2OCl_6]$, respectively (Willey *et al.*, 1993). Within the centrosymmetric cation unit $C_{14}H_{36}N_4{}^{4+}$, the C—C and N—C bond lengths vary from 1.520 (2) to 1.524 (2) Å and from 1.501 (2) to 1.513 (2) Å, respectively. The ranges of the N—C—C and C—N—C angles are 111.86 (15) to 116.39 (14)° and 108.81 (14) to 112.58 (14)°, respectively. The four nitrogen atoms of the macrocyclic cation are coplanar with the four nitrogens occupying the four corners of it with distances between each two N atoms of 3.2242 (13) Å (N1—N2), 5.414 (2) Å (N1—N1′) and 5.5907 (17) Å (N2—N2′), where the primed atoms are related by the symmetry operation $(-x + 1, -y + 1, -z)$. The bond lengths and angles within the tetraammonium organic cation are comparable to the corresponding values determined for the H_2TMC or H_4TMC moiety in $[H_2TMC][As_4O_2Cl_{10}]$, $[H_2TMC][Sb_2OCl_6]$ (Willey *et al.*, 1993), $[H_4TMC](ClO_4)_2Cl_2$ (Moon & Choi, 2020),

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N1—H1$\cdots$Cl2	0.99	2.16	3.120 (2)	163
N2—H2$\cdots$Cl2	0.99	2.08	3.0553 (17)	170
C2—H2A$\cdots$Cl2	0.98	2.85	3.642 (2)	139
C4—H4C$\cdots$O3	0.97	2.58	3.299 (4)	131
C5—H5AB$\cdots$Cl1	0.98	2.86	3.804 (2)	161
C3—H3A$\cdots$Cl2^i	0.98	2.72	3.541 (2)	142
C1—H1A$\cdots$Cl2^{ii}	0.98	2.74	3.511 (2)	136
C1—H1AB$\cdots$O1^{iii}	0.98	2.59	3.230 (3)	123
C2—H2AB$\cdots$O1^{iii}	0.98	2.54	3.047 (3)	112
C3—H3AB$\cdots$O1^{iii}	0.98	2.53	3.193 (3)	125
C4—H4A$\cdots$O3^{iv}	0.97	2.34	3.168 (3)	143
C5—H5A$\cdots$O3^{iv}	0.98	2.40	3.218 (3)	141
C7—H7B$\cdots$O3^{iv}	0.97	2.38	3.343 (3)	173
C4—H4B$\cdots$Cl1^v	0.97	2.88	3.773 (3)	154
C6—H6AB$\cdots$O2^{vi}	0.98	2.54	3.260 (3)	130

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

$[H_4TMC][H_2TMC][W(CN)_8]_2\cdot4H_2O$ (Nowicka *et al.*, 2012) and $[H_4TMC]_2[Sb_4F_{15}][HF_2]F_4$ (Becker & Mattes, 1996). The CrO_3Cl^- anion exhibits a more or less distorted tetrahedral geometry (Lorenzo Luis *et al.*, 1996). The O—Cr—O angles range from 110.49 (14) to 111.22 (13)° and the O—Cr—Cl angles from 108.34 (8) to 109.69 (10)°. The Cr—O bond distances range from 1.588 (2) to 1.602 (2) Å and Cr—Cl bond length is 2.200 (1) Å, in good agreement with the values (2.197 and 2.194 Å) reported for $Cs[CrO_3Cl]$ and $Rb[CrO_3Cl]$ (Foster & Sterns, 1974).

3. Supramolecular features

Extensive C—H$\cdots$O, C—H$\cdots$Cl and N—H$\cdots$Cl hydrogen-bonding interactions occur in the crystal structure (Table 1). The organic $C_{14}H_{36}N_4{}^{4+}$ cation is linked to two Cl$^-$ anions and one CrO_3Cl^- anion *via* N1—H1$\cdots$Cl2, N2—H2$\cdots$Cl2 and C4—H4C$\cdots$O3 hydrogen bonds, respectively. In addition, three neighbouring organic cations are interconnected to the
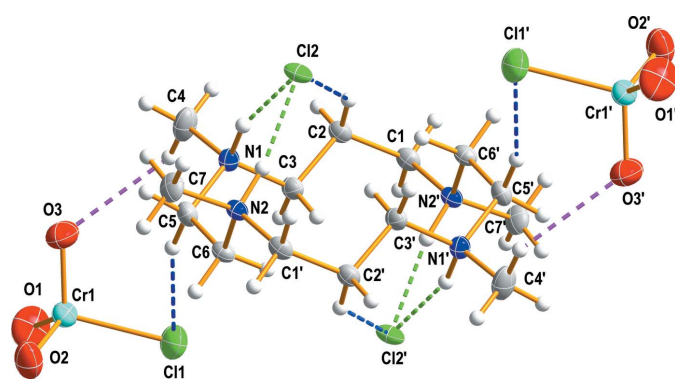

Figure 1
The structure of (I), drawn with displacement ellipsoids at the 50% probability level. Dashed lines represent hydrogen bonding interactions and primed atoms are related by the symmetry operation $(-x + 1, -y + 1, -z)$.
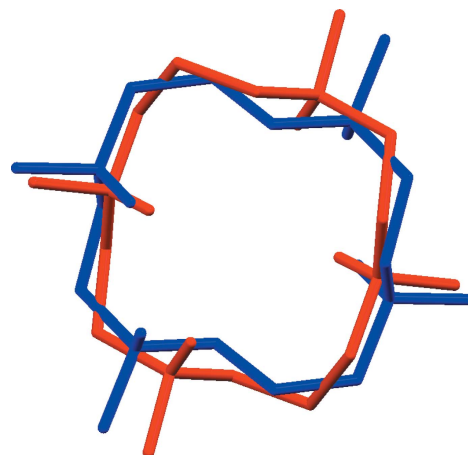
Figure 2
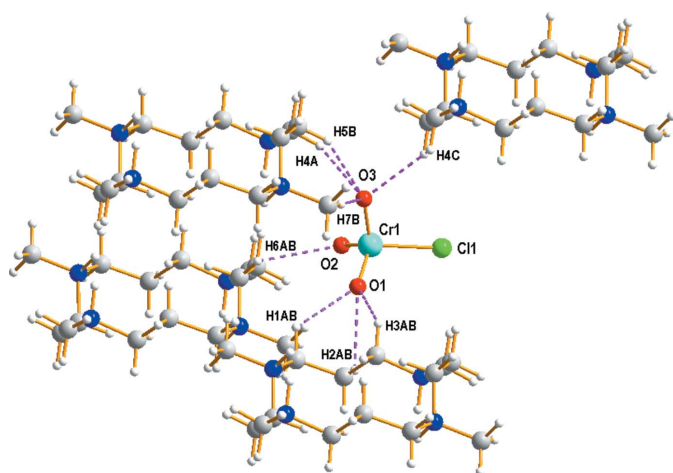Overlay of the two macrocyclic cations in (I) (blue) and in $[H_4TMC](ClO_4)_2Cl_2$ (red).

Figure 3
The C—H···O hydrogen-bonding interactions between neighbouring organic cations and the CrO₃Cl⁻ anion (see Table 1 for details).

CrO₃Cl⁻ anion *via* several C—H···O hydrogen bonds (Fig. 3). The extensive array of these contacts generates a three-dimensional network and help to consolidate the crystal structure. The crystal packing diagram of (I) viewed perpendicular to the *bc* plane is shown in Fig. 4.

4. Database survey

A search of the Cambridge Structural Database (Version 5.41, November 2019; Groom *et al.*, 2016) indicated only seven hits for organic compounds containing C₁₄H₃₂N₄, C₁₄H₃₄N₄²⁺ or C₁₄H₃₆N₄⁴⁺ macrocycles: C₁₄H₃₂N₄ (refcode LEPXOT; Willey *et al.*, 1994), [Ga₂(C₃H₇)₄(OH)₂](C₁₄H₃₂N₄) (XEGGUL; Boag *et al.*, 2000), Mg₃Al₁₃P₁₆O₆₄·1.5(C₁₄H₃₂N₄)·· 2.5H₂O (DAWQUN; Patinec *et al.*, 1999), [C₁₄H₃₆N₄]₂[Sb₄F₁₅]- [HF₂]F₄ (ZITQUO; Becker *et al.*, 1996), [C₁₄H₃₄N₄]-
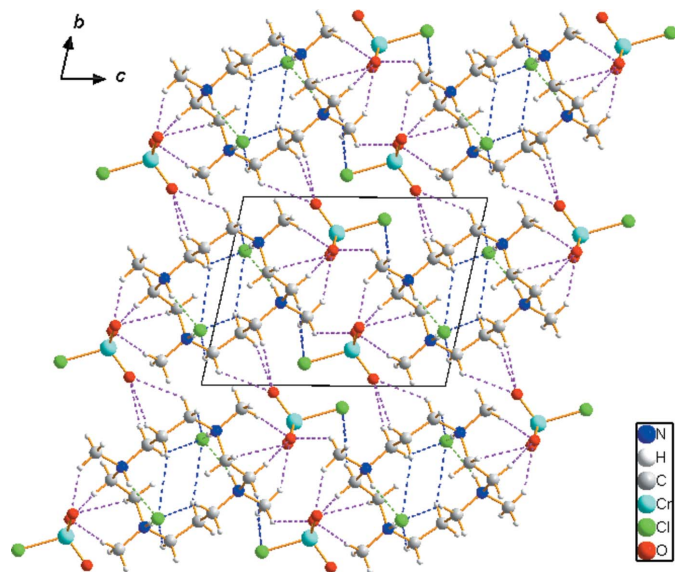

Figure 4
The crystal packing of (I), viewed perpendicular to the *bc* plane. Dashed lines represent N—H···Cl (green), C—H···O (pink) and C—H···Cl (blue) hydrogen-bonding interactions (see Table 1 for details).

Table 2
Experimental details.

Crystal data	
Chemical formula	(C₁₄H₃₆N₄)[CrO₃Cl]₂Cl₂
M_r	602.27
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	220
a, b, c (Å)	7.0610 (14), 8.6740 (17), 10.775 (2)
α, β, γ (°)	77.61 (3), 88.20 (3), 79.39 (3)
V (Å³)	633.5 (2)
Z	1
Radiation type	Synchrotron, $\lambda = 0.610$ Å
μ (mm⁻¹)	0.85
Crystal size (mm)	0.21 × 0.15 × 0.11
Data collection	
Diffractometer	Rayonix MX225HS CCD area detector
Absorption correction	Empirical (using intensity measurements) (*HKL3000sm SCALEPACK*; Otwinowski & Minor, 1997)
T_{min}, T_{max}	0.552, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6933, 3503, 3357
R_{int}	0.022
$(\sin\theta/\lambda)_{max}$ (Å⁻¹)	0.693
Refinement	
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.050, 0.150, 1.08
No. of reflections	3503
No. of parameters	138
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}, \Delta\rho_{min}$ (e Å⁻³)	0.81, −1.09

Computer programs: *PAL BL2D-SMDC* (Shin *et al.*, 2016), *HKL3000sm* (Otwinowski & Minor, 1997), *SHELXT2018* (Sheldrick, 2015a), *SHELXL2018* (Sheldrick, 2015b), *DIAMOND4* (Putz & Brandenburg, 2014) and *publCIF* (Westrip, 2010).

[As₄O₂Cl₁₀] (YALNII; Willey *et al.*, 1993), [C₁₄H₃₄N₄]- [Sb₂OCl₆] (YALNEE; Willey *et al.*, 1993) and [C₁₄H₃₆N₄]- [C₁₄H₃₄N₄][W(CN)₈]₂·4H₂O (ACIKUU; Nowicka *et al.*, 2012). The conformation of the organic C₁₄H₃₆N₄⁴⁺ cation in (I) is comparable to the *trans*-IV, *trans*-I and *trans*-III conformations of the macrocyclic cations in [C₁₄H₃₆N₄](ClO₄)₂Cl₂ (GUCVAE; Moon & Choi, 2020), [C₁₄H₃₄N₄][As₄O₂Cl₁₀] (YALNII), and [C₁₄H₃₄N₄][Sb₂OCl₆] (YALNEE), respectively. The *trans*-III and *trans*-IV conformations observed in the two crystallographically independent molecules of C₁₄H₃₂N₄ were also comparable (Willey *et al.*, 1994). However, the compound and structure of any double salt of C₁₄H₃₆N₄⁴⁺ with an additional CrClO₃⁻ anion is not yet known.

5. Synthesis and crystallization

The free macrocycle TMC (98%) and chromium(VI) trioxide (99%) were purchased from Sigma–Aldrich and used without further purification. All other chemicals were reagent-grade materials and used as received. To a solution of TMC (0.128 g, 0.5 mmol) in 6 *M* HCl (15 mL) was added a solution of chromium(VI) trioxide (0.1 g, 1 mmol) in 6 *M* HCl (5 mL) at 298 K. The resulting solution was stirred for 2 h and left to stand for slow evaporation at room temperature. Block-like red single crystals of (I) suitable for X-ray analysis were obtained by filtration.

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6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.97–0.98 Å and N—H = 0.99 Å, respectively, and with U_{iso}(H) values of 1.5 and $1.2U_{eq}$ of the parent atoms.

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Crystal structure of 1,4,8,11-tetramethyl-1,4,8,11-tetraazoniacyclotetradecane bis[chloridochromate(VI)] dichloride from synchrotron X-ray data

Dohyun Moon and Jong-Ha Choi

Computing details

Data collection: *PAL BL2D-SMDC* (Shin *et al.*, 2016); cell refinement: *HKL3000sm* (Otwinowski & Minor, 1997); data reduction: *HKL3000sm* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXT2018* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *DIAMOND4* (Putz & Brandenburg, 2014); software used to prepare material for publication: *publCIF* (Westrip, 2010).

1,4,8,11-Tetramethyl-1,4,8,11-tetraazoniacyclotetradecane bis[chloridochromate(VI)] dichloride

Crystal data

$(C_{14}H_{36}N_4)[CrO_3Cl]_2Cl_2$	$Z = 1$
$M_r = 602.27$	$F(000) = 312$
Triclinic, $P\bar{1}$	$D_x = 1.579$ Mg m^{-3}
$a = 7.0610$ (14) Å	Synchrotron radiation, $\lambda = 0.610$ Å
$b = 8.6740$ (17) Å	Cell parameters from 41622 reflections
$c = 10.775$ (2) Å	$\theta = 0.4–33.7°$
$\alpha = 77.61$ (3)°	$\mu = 0.85$ mm^{-1}
$\beta = 88.20$ (3)°	$T = 220$ K
$\gamma = 79.39$ (3)°	Block, red
$V = 633.5$ (2) Å^3	$0.21 \times 0.15 \times 0.11$ mm

Data collection

Rayonix MX225HS CCD area detector diffractometer	6933 measured reflections
Radiation source: PLSII 2D bending magnet	3503 independent reflections
ω scan	3357 reflections with $I > 2\sigma(I)$
Absorption correction: empirical (using intensity measurements) (*HKL3000sm Scalepack*; Otwinowski & Minor, 1997)	$R_{int} = 0.022$
	$\theta_{max} = 25.0°$, $\theta_{min} = 1.7°$
	$h = -9 \rightarrow 9$
	$k = -12 \rightarrow 12$
	$l = -14 \rightarrow 14$
$T_{min} = 0.552$, $T_{max} = 1.000$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.050$	$w = 1/[\sigma^2(F_o^2) + (0.1021P)^2 + 0.4428P]$
$wR(F^2) = 0.150$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	$(\Delta/\sigma)_{max} < 0.001$
3503 reflections	$\Delta\rho_{max} = 0.81$ e Å^{-3}
138 parameters	$\Delta\rho_{min} = -1.08$ e Å^{-3}
0 restraints	

Special details

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.5951 (2)	0.43908 (19)	0.24944 (14)	0.0197 (3)
H1	0.655924	0.528759	0.203398	0.024*
N2	0.3111 (2)	0.75634 (17)	0.10259 (15)	0.0178 (3)
H2	0.448197	0.736710	0.077822	0.021*
C1	0.8079 (3)	0.1708 (2)	0.01696 (18)	0.0203 (3)
H1A	0.942223	0.140900	−0.007767	0.024*
H1AB	0.763915	0.071671	0.058488	0.024*
C2	0.8030 (2)	0.2755 (2)	0.11389 (17)	0.0202 (3)
H2A	0.850838	0.373545	0.074404	0.024*
H2AB	0.889395	0.217967	0.184918	0.024*
C3	0.6013 (3)	0.3211 (2)	0.16488 (18)	0.0216 (3)
H3A	0.511705	0.368064	0.093415	0.026*
H3AB	0.559012	0.224125	0.212911	0.026*
C4	0.7083 (4)	0.3635 (3)	0.3696 (2)	0.0350 (5)
H4A	0.710246	0.443738	0.419628	0.052*
H4B	0.839127	0.320257	0.348638	0.052*
H4C	0.648561	0.277582	0.418098	0.052*
C5	0.3917 (3)	0.5084 (2)	0.28166 (17)	0.0214 (3)
H5A	0.398383	0.581772	0.338417	0.026*
H5AB	0.331618	0.420559	0.329015	0.026*
C6	0.2612 (2)	0.5985 (2)	0.16973 (17)	0.0191 (3)
H6A	0.265642	0.529620	0.108100	0.023*
H6AB	0.128516	0.617792	0.200171	0.023*
C7	0.2870 (3)	0.8760 (2)	0.1871 (2)	0.0287 (4)
H7A	0.309296	0.978749	0.138299	0.043*
H7B	0.378911	0.838265	0.256843	0.043*
H7C	0.157143	0.888100	0.220467	0.043*
Cr1	0.20005 (5)	0.19152 (4)	0.58525 (3)	0.02581 (14)
Cl1	0.21038 (11)	0.11680 (9)	0.40216 (7)	0.04726 (19)
O1	0.2178 (4)	0.0382 (3)	0.6983 (2)	0.0578 (6)
O2	0.0005 (3)	0.3102 (3)	0.59266 (19)	0.0461 (5)
O3	0.3790 (3)	0.2812 (3)	0.5855 (2)	0.0459 (5)
Cl2	0.74460 (6)	0.71108 (6)	0.05475 (5)	0.02599 (15)

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0203 (7)	0.0201 (7)	0.0179 (6)	−0.0016 (5)	−0.0003 (5)	−0.0042 (5)
N2	0.0161 (6)	0.0139 (6)	0.0231 (7)	−0.0019 (5)	0.0036 (5)	−0.0049 (5)

C1	0.0175 (7)	0.0155 (7)	0.0252 (8)	0.0018 (6)	0.0016 (6)	−0.0024 (6)
C2	0.0168 (7)	0.0194 (8)	0.0226 (8)	−0.0002 (6)	0.0009 (6)	−0.0030 (6)
C3	0.0189 (8)	0.0223 (8)	0.0244 (8)	−0.0023 (6)	0.0029 (6)	−0.0085 (6)
C4	0.0384 (12)	0.0407 (12)	0.0216 (9)	0.0067 (9)	−0.0102 (8)	−0.0078 (8)
C5	0.0220 (8)	0.0216 (8)	0.0192 (7)	−0.0018 (6)	0.0050 (6)	−0.0038 (6)
C6	0.0174 (7)	0.0155 (7)	0.0239 (8)	−0.0034 (5)	0.0041 (6)	−0.0030 (6)
C7	0.0381 (11)	0.0196 (8)	0.0312 (9)	−0.0048 (7)	0.0047 (8)	−0.0124 (7)
Cr1	0.0292 (2)	0.0227 (2)	0.0242 (2)	−0.00618 (13)	0.00070 (13)	−0.00076 (13)
Cl1	0.0520 (4)	0.0530 (4)	0.0450 (4)	−0.0119 (3)	0.0076 (3)	−0.0274 (3)
O1	0.0855 (18)	0.0349 (10)	0.0450 (11)	−0.0130 (10)	−0.0045 (11)	0.0111 (8)
O2	0.0433 (10)	0.0534 (11)	0.0367 (9)	0.0066 (9)	0.0027 (7)	−0.0126 (8)
O3	0.0468 (11)	0.0535 (12)	0.0454 (10)	−0.0246 (9)	−0.0010 (8)	−0.0141 (9)
Cl2	0.0172 (2)	0.0255 (2)	0.0356 (3)	−0.00824 (16)	0.00510 (17)	−0.00431 (19)

Geometric parameters (Å, º)

N1—C4	1.501 (2)	C4—H4A	0.9700
N1—C3	1.503 (2)	C4—H4B	0.9700
N1—C5	1.511 (2)	C4—H4C	0.9700
N1—H1	0.9900	C5—C6	1.521 (3)
N2—C6	1.503 (2)	C5—H5A	0.9800
N2—C7	1.505 (2)	C5—H5AB	0.9800
N2—C1^i	1.513 (2)	C6—H6A	0.9800
N2—H2	0.9900	C6—H6AB	0.9800
C1—C2	1.520 (3)	C7—H7A	0.9700
C1—H1A	0.9800	C7—H7B	0.9700
C1—H1AB	0.9800	C7—H7C	0.9700
C2—C3	1.524 (2)	Cr1—O1	1.588 (2)
C2—H2A	0.9800	Cr1—O2	1.596 (2)
C2—H2AB	0.9800	Cr1—O3	1.602 (2)
C3—H3A	0.9800	Cr1—Cl1	2.2000 (9)
C3—H3AB	0.9800		
C4—N1—C3	110.93 (15)	N1—C4—H4A	109.5
C4—N1—C5	109.63 (15)	N1—C4—H4B	109.5
C3—N1—C5	112.58 (14)	H4A—C4—H4B	109.5
C4—N1—H1	107.8	N1—C4—H4C	109.5
C3—N1—H1	107.8	H4A—C4—H4C	109.5
C5—N1—H1	107.8	H4B—C4—H4C	109.5
C6—N2—C7	112.00 (15)	N1—C5—C6	116.12 (14)
C6—N2—C1^i	112.21 (14)	N1—C5—H5A	108.3
C7—N2—C1^i	108.81 (14)	C6—C5—H5A	108.3
C6—N2—H2	107.9	N1—C5—H5AB	108.3
C7—N2—H2	107.9	C6—C5—H5AB	108.3
C1^i—N2—H2	107.9	H5A—C5—H5AB	107.4
N2^i—C1—C2	116.39 (14)	N2—C6—C5	115.04 (15)
N2^i—C1—H1A	108.2	N2—C6—H6A	108.5
C2—C1—H1A	108.2	C5—C6—H6A	108.5

N2^i—C1—H1AB	108.2	N2—C6—H6AB	108.5
C2—C1—H1AB	108.2	C5—C6—H6AB	108.5
H1A—C1—H1AB	107.3	H6A—C6—H6AB	107.5
C1—C2—C3	112.61 (15)	N2—C7—H7A	109.5
C1—C2—H2A	109.1	N2—C7—H7B	109.5
C3—C2—H2A	109.1	H7A—C7—H7B	109.5
C1—C2—H2AB	109.1	N2—C7—H7C	109.5
C3—C2—H2AB	109.1	H7A—C7—H7C	109.5
H2A—C2—H2AB	107.8	H7B—C7—H7C	109.5
N1—C3—C2	111.86 (15)	O1—Cr1—O2	110.49 (14)
N1—C3—H3A	109.2	O1—Cr1—O3	111.05 (14)
C2—C3—H3A	109.2	O2—Cr1—O3	111.22 (13)
N1—C3—H3AB	109.2	O1—Cr1—Cl1	109.69 (10)
C2—C3—H3AB	109.2	O2—Cr1—Cl1	108.34 (8)
H3A—C3—H3AB	107.9	O3—Cr1—Cl1	105.90 (9)
N2^i—C1—C2—C3	61.3 (2)	C3—N1—C5—C6	−59.5 (2)
C4—N1—C3—C2	−67.1 (2)	C7—N2—C6—C5	−64.42 (19)
C5—N1—C3—C2	169.64 (15)	C1^i—N2—C6—C5	172.85 (14)
C1—C2—C3—N1	−173.71 (14)	N1—C5—C6—N2	−69.9 (2)
C4—N1—C5—C6	176.52 (17)		

Symmetry code: (i) −x+1, −y+1, −z.

Hydrogen-bond geometry (Å, º)

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N1—H1⋯Cl2	0.99	2.16	3.120 (2)	163
N2—H2⋯Cl2	0.99	2.08	3.0553 (17)	170
C2—H2*A*⋯Cl2	0.98	2.85	3.642 (2)	139
C4—H4*C*⋯O3	0.97	2.58	3.299 (4)	131
C5—H5*AB*⋯Cl1	0.98	2.86	3.804 (2)	161
C3—H3*A*⋯Cl2^i	0.98	2.72	3.541 (2)	142
C1—H1*A*⋯Cl2^{ii}	0.98	2.74	3.511 (2)	136
C1—H1*AB*⋯O1^{iii}	0.98	2.59	3.230 (3)	123
C2—H2*AB*⋯O1^{iii}	0.98	2.54	3.047 (3)	112
C3—H3*AB*⋯O1^{iii}	0.98	2.53	3.193 (3)	125
C4—H4*A*⋯O3^{iv}	0.97	2.34	3.168 (3)	143
C5—H5*A*⋯O3^{iv}	0.98	2.40	3.218 (3)	141
C7—H7*B*⋯O3^{iv}	0.97	2.38	3.343 (3)	173
C4—H4*B*⋯Cl1^v	0.97	2.88	3.773 (3)	154
C6—H6*AB*⋯O2^{vi}	0.98	2.54	3.260 (3)	130

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