Acta Cryst E
CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Crystal structure of 1,4-bis(3-ammoniopropyl)-piperazine-1,4-diium bis[dichromate(VI)]

S. Vetrivel,[a] E. Vinoth,[a] R. U. Mullai,[a] R. Aruljothi[a] and M. NizamMohideen[b]*

[a]PG & Research Department of Physics, Government Arts College, Tiruvannamalai 606 603, Tamil Nadu, India, and [b]Department of Physics, The New College (Autonomous), Chennai 600 014, Tamil Nadu, India. *Correspondence e-mail: mnizam_new@yahoo.in

Received 9 March 2016
Accepted 29 March 2016

Edited by M. Weil, Vienna University of Technology, Austria

Keywords: crystal structure; dichromate anion; piperazinediium cation; molecular salt; hydrogen bonding..

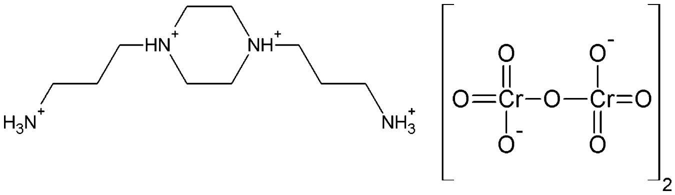
CCDC reference: 1471068

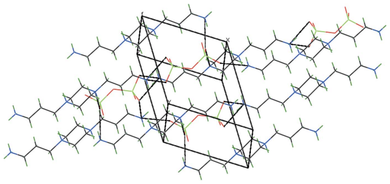
Supporting information: this article has supporting information at journals.iucr.org/e

The asymmetric unit of the organic–inorganic title salt, $(C_{10}H_{28}N_4)[Cr_2O_7]_2$, comprises one half of an 1,4-bis(3-ammoniopropyl)piperazinediium cation (the other half being generated by the application of inversion symmetry) and a dichromate anion. The piperazine ring of the cation adopts a chair conformation, and the two CrO_4 tetrahedra of the anion are in an almost eclipsed conformation. In the crystal, the cations and anions form a layered arrangement parallel to (001). N—H···O hydrogen bonds between the cations and anions and additional C—H···O interactions lead to the formation of a three-dimensional network structure.

1. Chemical context

Chromium is usually found in trivalent and hexavalent oxidation states in soil, ground water and seawater (Cespón-Romero *et al.*, 1996). Trivalent chromium is an essential element in mammals for maintaining efficient glucose, lipid and protein metabolism. On the other hand, hexavalent chromium is toxic and recognized as a carcinogen to humans and wildlife. Hence the dichromate ion is environmentally important due to its high toxicity (Yusof & Malek, 2009) and its use in many industrial processes (Goyal *et al.*, 2003). Recently, the reactions between hexaureachromium(III) and inorganic oxoanions (such as $Cr_2O_7^{2-}$ or CrO_4^{2-}) in aqueous solution have been investigated (Moon *et al.*, 2015). Numerous piperazine derivatives have shown a wide spectrum of biological activities, *viz.* antibacterial (Foroumadi *et al.*, 2007), antifungal (Upadhayaya *et al.*, 2004), anticancer (Chen *et al.*, 2006), antiparasitic (Cunico *et al.*, 2009), antihistamine (Smits *et al.*, 2008) or antidepressive activities (Becker *et al.*, 2006). Antidiabetic, anti-inflammatory, antitubercular, antimalarial, anticonvulsant, antipyretic, antitumor, anthelmintic and analgesic activities (Gan *et al.*, 2009*a*,*b*; Willems & Ilzerman, 2010) have also been found to be caused by this versatile moiety. In view of these important properties, we have undertaken the synthesis and X-ray diffraction study of the title compound.





OPEN ACCESS

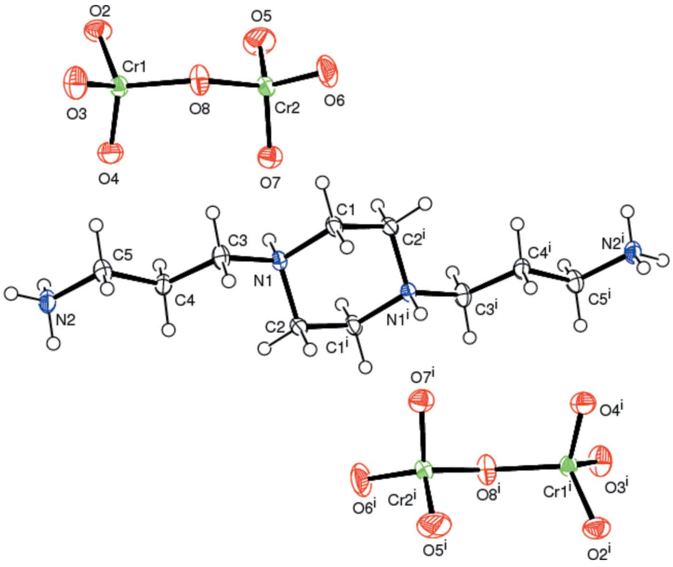


Figure 1
The entities of the organic–inorganic title salt. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $-x + 2, -y, -z + 1$.]

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1A···O3^{i}	0.97	2.28	3.176 (3)	152
C1—H1A···O4^{ii}	0.97	2.61	3.248 (3)	123
C1—H1B···O6	0.97	2.53	3.353 (3)	143
C2—H2A···O2^{iii}	0.97	2.49	3.298 (3)	141
C2—H2A···O4^{iii}	0.97	2.59	3.061 (3)	110
C2—H2B···O7^{iv}	0.97	2.59	3.232 (2)	124
C3—H3B···O3^{i}	0.97	2.58	3.383 (3)	140
C4—H4A···O5^{v}	0.97	2.38	3.208 (3)	143
C4—H4B···O7^{iii}	0.97	2.64	3.309 (2)	127
N2—H6A···O2^{vi}	0.89	2.18	3.040 (2)	161
N2—H6B···O7^{iii}	0.89	2.05	2.854 (2)	149
N2—H6C···O2^{v}	0.89	2.22	2.865 (2)	129
N2—H6C···O5^{iii}	0.89	2.64	3.239 (3)	125
N1—H1···O4^{iii}	0.98	2.43	3.113 (2)	126
N1—H1···O7	0.98	1.95	2.763 (2)	139

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

2. Structural commentary

The molecular entities of the title compound, consisting of a centrosymmetric 1,4-bis(3-ammoniopropyl)piperazinediium cation and a dichromate anion, are shown in Fig. 1. In the cation, the central piperazine ring (N1/C1/C2/N1^{i}/C1^{i}/C2^{i}; for symmetry operators, see Fig. 1) is substituted at the two N atoms by two ammoniopropyl moieties. The piperazine ring adopts a chair conformation, as is evident from the puckering parameters: $Q = 0.599$ (2) Å, $\tau = 180.0°$ and $\varphi = 0°$. Atoms N1 and N1^{i} are on opposite sides of the C1/C1^{i}/C2/C2^{i} plane and are both displaced from it by 0.2446 (19) Å. The chair conformation of the cation in the title structure is very similar to those of the same cation in the crystal structures of the 2-hydroxybenzoate (Cukrowski *et al.*, 2012), the nitrate (Junk & Smith, 2005) and the tetrahydrogenpentaborate (Jiang *et al.*, 2009) salts, despite the differences in the size and shape of the anions in the various structures. The tetrahedral CrO_4 groups in the anion of the title structure are fused together by a common O atom (O8) and are in an almost eclipsed conformation (Brandon & Brown, 1968). The Cr—O bond lengths follow the characteristic distribution for dichromate anions, with two longer bridging Cr—O bonds of 1.7676 (16) and 1.7746 (15) Å and six shorter terminal Cr—O bonds [range 1.5909 (19)–1.6185 (15) Å]. The Cr1—O8—Cr2 bridging angle in the complex anion is 127.48 (10)°. The tetrahedral O—Cr—O bond angles [range 106.52 (8) to 112.85 (12)°] indicate slight angular distortions.

3. Supramolecular features

The organic cations and inorganic anions are each arranged in rows parallel to [100] and alternate with each other along

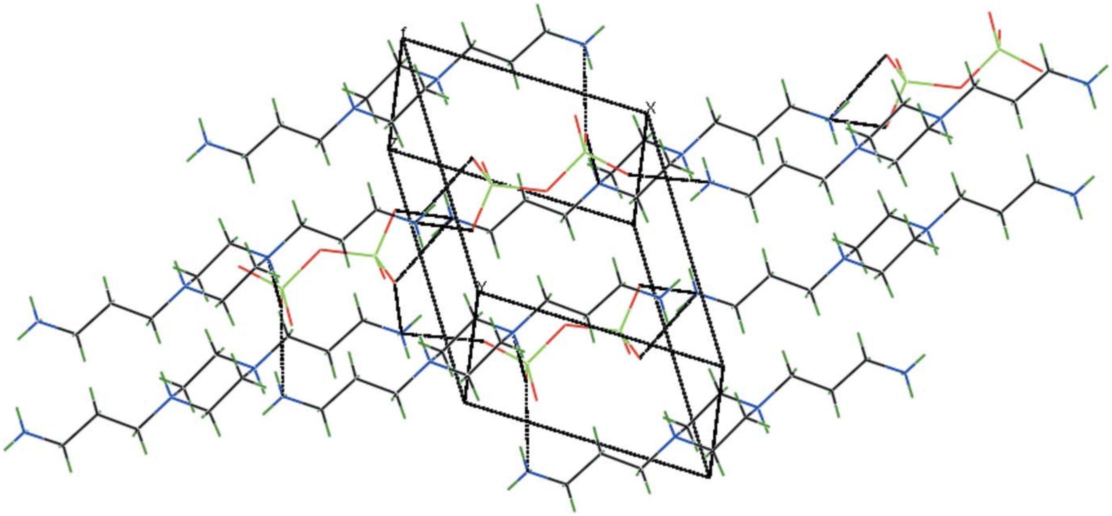


Figure 2
The packing of the molecular entities in the crystal structure of the title salt.

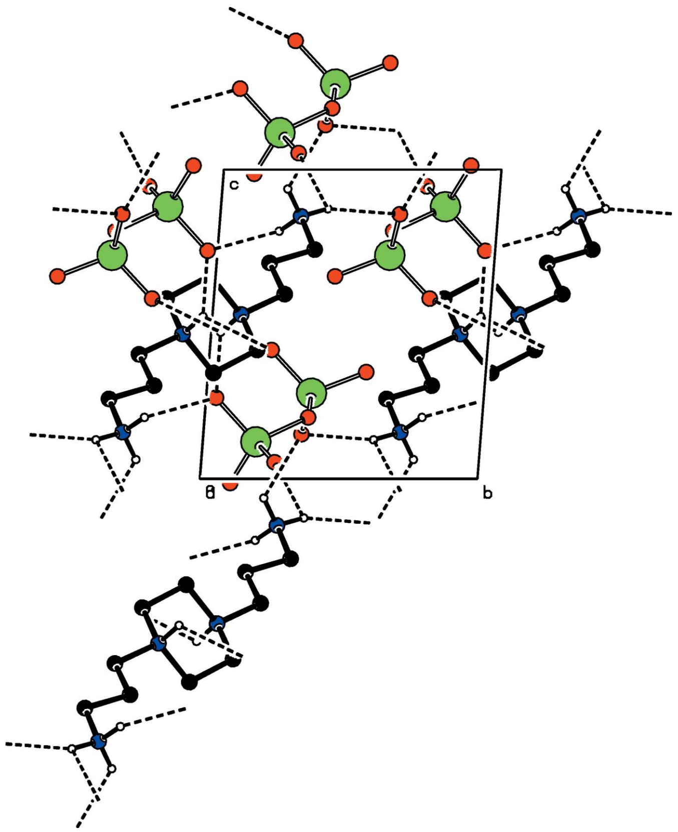


Figure 3
A part of the crystal structure of the title salt in a view along [100] showing N—H···O hydrogen-bonding interactions as dashed lines. C—H···O interactions are omitted for clarity.

[010], forming a layered arrangement parallel to (001). N—H···O hydrogen bonds (Table 1) between the cations, involving both primary and tertiary ammonium groups, and the anions lead to a three-dimensional network structure (Figs. 2 and 3). Additional C—H···O interactions consolidate this arrangement.

4. Synthesis and crystallization

Potassium dichromate and 1,4-bis(3-aminopropyl)piperazine (PDBP) were mixed in a molar ratio of 2:1 in water. Potassium dichromate was first dissolved in Millipore water of 18.2 MΩ·cm resistivity. Then the amount of PDBP was slowly added to the solution together with a few drops of concentrated hydrochloric acid and the mixture stirred for 18 h. The solution was then filtered twice with Wattmann filter paper and poured into petri dishes to evaporate at room temperature for several days. Recrystallization from water improved the quality of the material and increased the size of the crystals (maximum crystal size $5 \times 3 \times 2$ mm^3 after 35 d). A specimen was cleaved for the present structure determination.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All hydrogen atoms were placed geometrically and refined using a riding model: N—H = 0.89 Å for the primary ammonium group with U_{iso}(H) = 1.5U_{eq}(N); N—H = 0.98 Å for the tertiary ammonium group with U_{iso}(H) = 1.2U_{eq}(N); C—H = 0.97 Å with U_{iso}(H) = 1.2U_{eq}(C).

Table 2
Experimental details.

Crystal data	
Chemical formula	$(C_{10}H_{28}N_4)[Cr_2O_7]_2$
M_r	636.36
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	293
a, b, c (Å)	8.5361 (3), 8.6272 (3), 8.8576 (3)
α, β, γ (°)	77.761 (1), 72.307 (1), 60.985 (1)
V (Å^3)	541.81 (3)
Z	1
Radiation type	Mo $K\alpha$
μ (mm^{-1})	2.03
Crystal size (mm)	0.35 × 0.30 × 0.25
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.528, 0.649
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10263, 1913, 1835
R_{int}	0.020
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.023, 0.068, 1.06
No. of reflections	1913
No. of parameters	145
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.44, −0.45

Computer programs: *APEX2* and *SAINT* (Bruker, 2004), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014/7* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* and *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

Acknowledgements

The authors are grateful to the SAIF, IIT, Madras, India, for the data collection.

References

Becker, O. M., Dhanoa, D. S., Marantz, Y., Chen, D., Shacham, S., Cheruku, S., Heifetz, A., Mohanty, P., Fichman, M., Sharadendu, A., Nudelman, R., Kauffman, M. & Noiman, S. (2006). *J. Med. Chem.* **49**, 3116–3135.
Brandon, J. K. & Brown, I. D. (1968). *Can. J. Chem.* **46**, 933–941.
Bruker (2004). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cespón-Romero, R. M., Yebra-Biurrun, M. C. & Bermejo-Barrera, M. P. (1996). *Anal. Chim. Acta*, **327**, 37–45.
Chen, J. J., Lu, M., Jing, Y. K. & Dong, J. H. (2006). *Bioorg. Med. Chem.* **14**, 6539–6547.
Cukrowski, I., Adeyinka, A. S. & Liles, D. C. (2012). *Acta Cryst.* E**68**, o2387.
Cunico, W., Gomes, C. R. B., Moreth, M., Manhanini, D. P., Figueiredo, I. H., Penido, C., Henriques, M. G. M. O., Varotti, F. P. & Krettli, A. U. (2009). *Eur. J. Med. Chem.* **44**, 1363–1368.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Foroumadi, A., Emami, S., Mansouri, S., Javidnia, A., Saeid-Adeli, N., Shirazi, F. H. & Shafiee, A. (2007). *Eur. J. Med. Chem.* **42**, 985–992.

Gan, L. L., Cai, J. L. & Zhou, C. H. (2009*a*). *Chin. Pharm. J.* **44**, 1361–1368.

Gan, L. L., Lu, Y. H. & Zhou, C. H. (2009*b*). *Chin. J. Biochem. Pharm*. **30**, 127–131.

Goyal, N., Jain, S. C. & Banerjee, U. C. (2003). *Adv. Environ. Res.* **7**, 311–319.

Jiang, X., Liu, H.-X., Wu, S.-L. & Liang, Y.-X. (2009). *Jiegou Huaxue (Chin. J. Struct. Chem.)*, **28**, 723–729.

Junk, P. C. & Smith, M. K. (2005). *C. R. Chim.* **8**, 189–198.

Moon, D., Tanaka, S., Akitsu, T. & Choi, J.-H. (2015). *Acta Cryst.* E**71**, 1336–1339.

Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.

Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

Smits, R. A., Lim, H. D., Hanzer, A., Zuiderveld, O. P., Guaita, E., Adami, M., Coruzzi, G., Leurs, R. & de Esch, I. J. P. (2008). *J. Med. Chem.* **51**, 2457–2467.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Upadhayaya, R. S., Sinha, N., Jain, S., Kishore, N., Chandra, R. & Arora, S. K. (2004). *Bioorg. Med. Chem.* **12**, 2225–2238.

Willems, L. I. & Ilzerman, A. P. (2010). *Med. Chem. Res*. **30**, 778–817.

Yusof, A. M. & Malek, N. A. N. N. (2009). *J. Hazard. Mater.* **162**, 1019–1024.

supporting information

Acta Cryst. (2016). E**72**, 616-619   [doi:10.1107/S2056989016005284]

Crystal structure of 1,4-bis(3-ammoniopropyl)piperazine-1,4-diium bis[dichromate(VI)]

S. Vetrivel, E. Vinoth, R. U. Mullai, R. Aruljothi and M. NizamMohideen

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: SHELXT (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2014*/7 (Sheldrick, 2015*b*); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 2012) and *PLATON* (Spek, 2009).

1,4-Bis(3-ammoniopropyl)piperazine-1,4-diium bis[dichromate(VI)]

Crystal data

$(C_{10}H_{28}N_4)[Cr_2O_7]_2$
$M_r = 636.36$
Triclinic, $P\overline{1}$
$a = 8.5361$ (3) Å
$b = 8.6272$ (3) Å
$c = 8.8576$ (3) Å
$\alpha = 77.761$ (1)°
$\beta = 72.307$ (1)°
$\gamma = 60.985$ (1)°
$V = 541.81$ (3) Å^3

$Z = 1$
$F(000) = 324$
$D_x = 1.950$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9982 reflections
$\theta = 2.4$–39.1°
$\mu = 2.03$ mm^{-1}
$T = 293$ K
Needle, brown
0.35 × 0.30 × 0.25 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min} = 0.528$, $T_{max} = 0.649$

10263 measured reflections
1913 independent reflections
1835 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.4°$
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -10 \rightarrow 10$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.068$
$S = 1.06$
1913 reflections
145 parameters
0 restraints

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2 + 0.4739P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ e Å^{-3}

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 (Å²)

	x	y	z	$U_{\rm iso}$*/$U_{\rm eq}$
C1	0.9278 (3)	0.1703 (3)	0.4169 (2)	0.0217 (4)
H1A	0.9548	0.2371	0.4721	0.026*
H1B	0.8679	0.2498	0.3344	0.026*
C2	0.8955 (3)	−0.0195 (3)	0.6574 (2)	0.0209 (4)
H2A	0.8158	−0.0661	0.7319	0.025*
H2B	0.9217	0.0454	0.7154	0.025*
C3	0.6197 (3)	0.2538 (3)	0.5974 (3)	0.0247 (4)
H3A	0.5710	0.3344	0.5101	0.030*
H3B	0.6391	0.3191	0.6608	0.030*
C4	0.4805 (3)	0.1911 (3)	0.6986 (2)	0.0218 (4)
H4A	0.5194	0.1252	0.7946	0.026*
H4B	0.4723	0.1127	0.6407	0.026*
C5	0.2943 (3)	0.3494 (3)	0.7415 (3)	0.0259 (4)
H5A	0.3046	0.4315	0.7931	0.031*
H5B	0.2522	0.4109	0.6457	0.031*
N2	0.1592 (2)	0.2910 (2)	0.8492 (2)	0.0261 (4)
H6A	0.0501	0.3852	0.8736	0.039*
H6B	0.1488	0.2168	0.8012	0.039*
H6C	0.1973	0.2358	0.9376	0.039*
N1	0.8006 (2)	0.1028 (2)	0.53184 (19)	0.0183 (3)
H1	0.7772	0.0338	0.4742	0.022*
O2	0.1839 (2)	0.3536 (2)	0.14426 (19)	0.0359 (4)
O3	0.1272 (2)	0.5696 (2)	0.3451 (2)	0.0402 (4)
O4	0.2800 (2)	0.2224 (2)	0.41686 (19)	0.0359 (4)
O5	0.6705 (3)	0.1105 (3)	−0.0133 (2)	0.0612 (6)
O6	0.8440 (3)	0.2646 (3)	0.0538 (3)	0.0564 (6)
O7	0.7517 (2)	0.0359 (2)	0.26223 (19)	0.0325 (4)
O8	0.4835 (2)	0.3730 (2)	0.1987 (2)	0.0370 (4)
Cr1	0.26337 (4)	0.37840 (4)	0.27693 (4)	0.02227 (12)
Cr2	0.69282 (5)	0.19141 (5)	0.11987 (4)	0.02748 (13)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0192 (10)	0.0226 (9)	0.0222 (10)	−0.0120 (8)	−0.0008 (8)	0.0007 (8)
C2	0.0202 (10)	0.0260 (10)	0.0166 (9)	−0.0124 (8)	−0.0013 (7)	−0.0014 (8)
C3	0.0179 (10)	0.0213 (10)	0.0303 (11)	−0.0073 (8)	0.0011 (8)	−0.0071 (8)
C4	0.0157 (9)	0.0230 (10)	0.0246 (10)	−0.0080 (8)	−0.0029 (8)	−0.0026 (8)
C5	0.0200 (10)	0.0246 (10)	0.0281 (11)	−0.0088 (8)	0.0008 (8)	−0.0051 (8)

N2	0.0163 (8)	0.0313 (9)	0.0275 (9)	−0.0091 (7)	−0.0014 (7)	−0.0056 (7)
N1	0.0155 (8)	0.0201 (8)	0.0190 (8)	−0.0087 (7)	−0.0006 (6)	−0.0042 (6)
O2	0.0460 (10)	0.0430 (9)	0.0291 (8)	−0.0252 (8)	−0.0145 (7)	−0.0021 (7)
O3	0.0322 (9)	0.0346 (9)	0.0514 (10)	−0.0121 (7)	−0.0011 (8)	−0.0190 (8)
O4	0.0387 (9)	0.0418 (9)	0.0313 (8)	−0.0217 (8)	−0.0124 (7)	0.0042 (7)
O5	0.0591 (13)	0.0843 (15)	0.0348 (10)	−0.0178 (12)	−0.0145 (9)	−0.0260 (10)
O6	0.0323 (10)	0.0645 (13)	0.0619 (13)	−0.0286 (9)	0.0011 (9)	0.0150 (10)
O7	0.0384 (9)	0.0356 (9)	0.0321 (8)	−0.0221 (7)	−0.0120 (7)	−0.0006 (7)
O8	0.0250 (8)	0.0364 (9)	0.0484 (10)	−0.0163 (7)	0.0005 (7)	−0.0085 (7)
Cr1	0.02026 (19)	0.0254 (2)	0.02321 (19)	−0.01134 (15)	−0.00346 (13)	−0.00582 (13)
Cr2	0.02130 (19)	0.0382 (2)	0.0210 (2)	−0.01414 (16)	−0.00041 (14)	−0.00334 (15)

Geometric parameters (Å, º)

C1—N1	1.498 (2)	C5—N2	1.478 (3)
C1—C2^{i}	1.502 (3)	C5—H5A	0.9700
C1—H1A	0.9700	C5—H5B	0.9700
C1—H1B	0.9700	N2—H6A	0.8900
C2—N1	1.493 (2)	N2—H6B	0.8900
C2—C1^{i}	1.502 (3)	N2—H6C	0.8900
C2—H2A	0.9700	N1—H1	0.9800
C2—H2B	0.9700	O2—Cr1	1.6185 (15)
C3—N1	1.498 (2)	O3—Cr1	1.6035 (16)
C3—C4	1.509 (3)	O4—Cr1	1.6070 (16)
C3—H3A	0.9700	O5—Cr2	1.5909 (19)
C3—H3B	0.9700	O6—Cr2	1.6068 (18)
C4—C5	1.511 (3)	O7—Cr2	1.6299 (16)
C4—H4A	0.9700	O8—Cr2	1.7676 (16)
C4—H4B	0.9700	O8—Cr1	1.7746 (15)
N1—C1—C2^{i}	111.02 (16)	C4—C5—H5B	109.6
N1—C1—H1A	109.4	H5A—C5—H5B	108.1
C2^{i}—C1—H1A	109.4	C5—N2—H6A	109.5
N1—C1—H1B	109.4	C5—N2—H6B	109.5
C2^{i}—C1—H1B	109.4	H6A—N2—H6B	109.5
H1A—C1—H1B	108.0	C5—N2—H6C	109.5
N1—C2—C1^{i}	110.02 (15)	H6A—N2—H6C	109.5
N1—C2—H2A	109.7	H6B—N2—H6C	109.5
C1^{i}—C2—H2A	109.7	C2—N1—C3	113.18 (15)
N1—C2—H2B	109.7	C2—N1—C1	108.55 (15)
C1^{i}—C2—H2B	109.7	C3—N1—C1	110.86 (15)
H2A—C2—H2B	108.2	C2—N1—H1	108.0
N1—C3—C4	112.22 (16)	C3—N1—H1	108.0
N1—C3—H3A	109.2	C1—N1—H1	108.0
C4—C3—H3A	109.2	Cr2—O8—Cr1	127.48 (10)
N1—C3—H3B	109.2	O3—Cr1—O4	110.80 (9)
C4—C3—H3B	109.2	O3—Cr1—O2	108.95 (9)
H3A—C3—H3B	107.9	O4—Cr1—O2	109.39 (8)

C3—C4—C5	109.66 (16)	O3—Cr1—O8	106.52 (8)
C3—C4—H4A	109.7	O4—Cr1—O8	108.31 (8)
C5—C4—H4A	109.7	O2—Cr1—O8	112.85 (9)
C3—C4—H4B	109.7	O5—Cr2—O6	112.85 (12)
C5—C4—H4B	109.7	O5—Cr2—O7	107.91 (11)
H4A—C4—H4B	108.2	O6—Cr2—O7	109.68 (9)
N2—C5—C4	110.30 (16)	O5—Cr2—O8	111.08 (10)
N2—C5—H5A	109.6	O6—Cr2—O8	106.39 (10)
C4—C5—H5A	109.6	O7—Cr2—O8	108.89 (8)
N2—C5—H5B	109.6		
N1—C3—C4—C5	−171.94 (16)	C2^{i}—C1—N1—C3	−176.16 (16)
C3—C4—C5—N2	−176.35 (16)	Cr2—O8—Cr1—O3	175.26 (12)
C1^{i}—C2—N1—C3	178.15 (15)	Cr2—O8—Cr1—O4	56.03 (15)
C1^{i}—C2—N1—C1	−58.3 (2)	Cr2—O8—Cr1—O2	−65.22 (15)
C4—C3—N1—C2	−64.5 (2)	Cr1—O8—Cr2—O5	52.36 (17)
C4—C3—N1—C1	173.31 (16)	Cr1—O8—Cr2—O6	175.53 (13)
C2^{i}—C1—N1—C2	58.9 (2)	Cr1—O8—Cr2—O7	−66.33 (14)

Symmetry code: (i) −*x*+2, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···O3^{ii}	0.97	2.28	3.176 (3)	152
C1—H1*A*···O4^{iii}	0.97	2.61	3.248 (3)	123
C1—H1*B*···O6	0.97	2.53	3.353 (3)	143
C2—H2*A*···O2^{iv}	0.97	2.49	3.298 (3)	141
C2—H2*A*···O4^{iv}	0.97	2.59	3.061 (3)	110
C2—H2*B*···O7^{i}	0.97	2.59	3.232 (2)	124
C3—H3*B*···O3^{ii}	0.97	2.58	3.383 (3)	140
C4—H4*A*···O5^{v}	0.97	2.38	3.208 (3)	143
C4—H4*B*···O7^{iv}	0.97	2.64	3.309 (2)	127
N2—H6*A*···O2^{vi}	0.89	2.18	3.040 (2)	161
N2—H6*B*···O7^{iv}	0.89	2.05	2.854 (2)	149
N2—H6*C*···O2^{v}	0.89	2.22	2.865 (2)	129
N2—H6*C*···O5^{iv}	0.89	2.64	3.239 (3)	125
N1—H1···O4^{iv}	0.98	2.43	3.113 (2)	126
N1—H1···O7	0.98	1.95	2.763 (2)	139

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