Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tris(morpholinium) hexa-μ_3-hydroxido-hexa-μ_2-oxido-dodecaoxidohexamolybdenum(VI)chromate(III) tetrahydrate

Yan-Yan Yang,[a] Yu Song,[b] Li-Ye Liu[a] and Xiao-Shu Qu[a]*

[a]Department of Chemistry and Pharmaceutical Engineering, Jilin Institute of Chemical Technology, Jilin 132022, People's Republic of China, and [b]Department of Animal Science, Jilin Agricultural Science and Technology College, Jilin 132101, People's Republic of China
Correspondence e-mail: xiaoshuqu@yahoo.com.cn

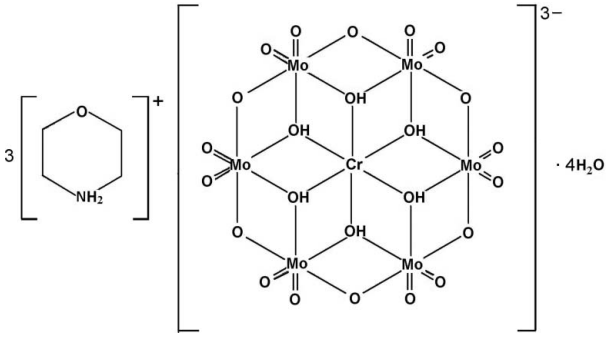
Received 3 May 2011; accepted 13 May 2011

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.008 Å; disorder in solvent or counterion; R factor = 0.026; wR factor = 0.082; data-to-parameter ratio = 13.0.

In the title organic–inorganic hybrid compound, $(C_4H_{10}NO)_3[H_6CrMo_6O_{24}]\cdot 4H_2O$, the Anderson-type $[H_6CrMo_6O_{24}]^{3-}$ polyoxoanion is centrosymmetric, with the Cr^{III} ion lying on an inversion center. One of the two crystallographiclly independent morpholinium cations is half-occupied. Intermolecular N—H···O and O—H···O hydrogen bonds link the cations, polyoxoanions and uncoordinated water molecules.

Related literature

For general background to the properties and applications of polyoxometalates, see: Hill (1998). For related compounds with Anderson-type polyoxometalate anions and organic cations, see: An *et al.* (2004); Wang *et al.* (2010). For synthetic details, see: Perloff (1970).



Experimental

Crystal data

$(C_4H_{10}NO)_3[H_6CrMo_6O_{24}]\cdot 4H_2O$
M_r = 1354.14
Triclinic, $P\overline{1}$
a = 7.9474 (4) Å
b = 9.9654 (5) Å
c = 13.7404 (7) Å
α = 110.392 (1)°
β = 102.921 (1)°
γ = 90.635 (1)°
V = 989.47 (9) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 2.20 mm^{-1}
T = 296 K
0.53 × 0.50 × 0.44 mm

Data collection

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.324, T_{max} = 0.380
5458 measured reflections
3855 independent reflections
3562 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.082
S = 1.09
3855 reflections
297 parameters
10 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O6^{i}	0.90	1.86	2.755 (4)	172
N1—H1B···O5	0.90	1.94	2.783 (4)	155
N2—H2C···O13^{ii}	0.90	2.19	2.976 (8)	145
N2—H2D···O2W^{iii}	0.90	2.53	3.294 (9)	144
O1—H1···O1W^{iv}	0.84 (1)	1.87 (1)	2.709 (4)	173 (5)
O2—H2···O2W^{iii}	0.85 (1)	1.80 (1)	2.640 (4)	172 (4)
O3—H3···O9^{v}	0.84 (1)	2.02 (1)	2.853 (4)	171 (5)
O1W—H7···O8^{vi}	0.84 (1)	2.08 (3)	2.837 (4)	148 (5)
O1W—H8···O10^{vi}	0.85 (1)	2.01 (2)	2.807 (5)	157 (5)
O2W—H4···O7	0.85 (1)	2.03 (2)	2.851 (4)	165 (5)
O2W—H5···O1W^{vii}	0.85 (1)	2.00 (2)	2.801 (5)	157 (4)

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2428).

References

An, H.-Y., Lan, Y., Li, Y.-G., Hao, N., Xiao, D.-R., Duan, L.-Y. & Xu, X. (2004). *Inorg. Chem. Commun.* **7**, 356–358.
Bruker (2007). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Hill, C. L. (1998). *Chem. Rev.* **98**, 1–2.
Perloff, A. (1970). *Inorg. Chem.* **9**, 2228–2239.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, S.-M., Chen, W.-L. & Wang, E.-B. (2010). *J. Clust. Sci.* **21**, 133–145.

supporting information

Acta Cryst. (2011). E**67**, m776 [doi:10.1107/S1600536811018149]

Tris(morpholinium) hexa-μ_3-hydroxido-hexa-μ_2-oxido-dodecaoxidohexamolybdenum(VI)chromate(III) tetrahydrate

Yan-Yan Yang, Yu Song, Li-Ye Liu and Xiao-Shu Qu

S1. Comment

It is known that the compounds containing molybdenum atoms, especially containing polyoxometalates and organic molecules, are good catalysts for oxidation reactions, because they can be applied as models for the interactions between organic substrates and catalytic metal oxide surfaces in heterogeneous catalysis employing solid molybdenum oxides (Hill, 1998). Herein, we report the structure of the title compound containning Anderson-type $[H_6CrMo_6O_{24}]^{3-}$ polyoxoanion, morpholinium cations and water molecules.

The title compound consists of one Anderson-type $[H_6CrMo_6O_{24}]^{3-}$ polyoxoanion (An *et al.*, 2004; Wang *et al.*, 2010), three morpholinium cations and four uncoordinated water molecules. The $[H_6CrMo_6O_{24}]^{3-}$ cluster with four different types of O atoms shows a classical B-type Anderson structure (Fig. 1), which made up of seven edge-sharing octahedra. Six $[MoO_6]$ octahedra are arranged hexagonally around one central $[Cr(OH)_6]$ octahedron. The Cr—O and Mo—O distances are normal. The molecules are linked into a three-dimensional network by a combination of intermolecular N—H···O and O—H···O hydrogen bonds (Table 1).

S2. Experimental

The title compound was synthesized by mixing $CrCl_3.6H_2O$ (0.266 g, 1 mmol), $Na_2MoO_4.2H_2O$ (1.464 g, 6 mmol) and morpholine (1.80 g, 1.2 mmol) in H_2O (50 ml) and boiling the mixture (Perloff, 1970). The pH value of the solution was adjusted to 1.0 by addition of 1 *M* hydrochloric acid. The mixture was refluxed for 2 h, and then the solution was cooled to room temperature. After two days, pink block crystals were formed by evaporation of the filtrate at room temperature.

S3. Refinement

H atoms on C and N atoms were positioned geometrically and refined as riding atoms, with C—H = 0.97, N—H = 0.90 Å and U_{iso}(H) = 1.2U_{eq}(C, N). Water H atoms were located in a difference Fourier map and refined isotropically, with O—H distance restraints of 0.85 (1) Å. The highest residual electron density was found at 0.65 Å from H6A atom and the deepest hole at 0.88 Å from Mo3 atom.

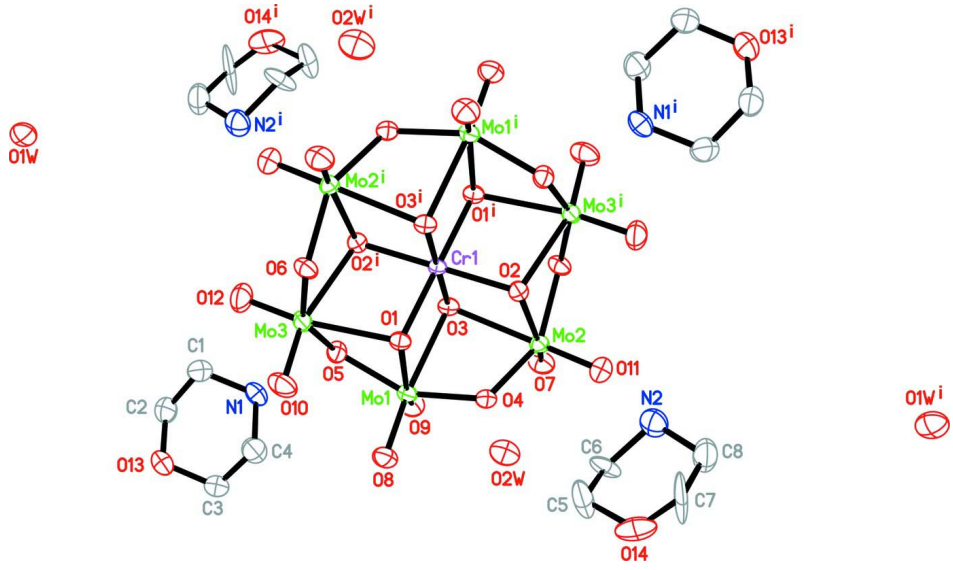


Figure 1

The structure of the title compound, with displacement ellipsoids drawn at the 50% probability level. The morpholinium cation containing N2 is half-occupied. H atoms have been omitted for clarity. [Symmetry code: (i) -x, -y, -z.]

Tris(morpholinium) hexa-μ_3-hydroxido-hexa-μ_2-oxido- dodecaoxidohexamolybdenum(VI)chromate(III) tetrahydrate

Crystal data

$(C_4H_{10}NO)_3[H_6CrMo_6O_{24}]\cdot 4H_2O$
$M_r = 1354.14$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.9474\ (4)$ Å
$b = 9.9654\ (5)$ Å
$c = 13.7404\ (7)$ Å
$\alpha = 110.392\ (1)°$
$\beta = 102.921\ (1)°$
$\gamma = 90.635\ (1)°$
$V = 989.47\ (9)$ Å^3
$Z = 1$
$F(000) = 661$
$D_x = 2.273$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3855 reflections
$\theta = 2.8–26.1°$
$\mu = 2.20$ mm^{-1}
$T = 296$ K
Block, pink
0.53 × 0.50 × 0.44 mm

Data collection

Bruker APEX CCD diffractometer
Radiation source: sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.324$, $T_{max} = 0.380$
5458 measured reflections
3855 independent reflections
3562 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 26.1°$, $\theta_{min} = 1.6°$
$h = -9\rightarrow 9$
$k = -10\rightarrow 12$
$l = -16\rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.082$
$S = 1.09$
3855 reflections
297 parameters
10 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0428P)^2 + 2.0824P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.18$ e Å^{-3}
$\Delta\rho_{min} = -0.55$ e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0147 (6)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.0340 (3)	0.2032 (3)	0.0153 (2)	0.0204 (5)	
O13	0.7910 (5)	0.7096 (3)	0.3943 (3)	0.0447 (8)	
O2	−0.0919 (3)	−0.0753 (3)	−0.1564 (2)	0.0205 (5)	
O1W	0.8003 (5)	0.3343 (3)	0.9120 (3)	0.0412 (7)	
O3	0.2284 (3)	−0.0122 (3)	−0.0349 (2)	0.0198 (5)	
O2W	0.6478 (4)	0.0583 (4)	−0.2236 (3)	0.0446 (8)	
O4	0.1684 (3)	0.1183 (3)	−0.1629 (2)	0.0248 (6)	
O5	0.3302 (3)	0.2637 (3)	0.1333 (2)	0.0243 (5)	
O6	−0.0971 (3)	0.2717 (3)	0.2074 (2)	0.0252 (6)	
O7	0.3543 (4)	−0.1184 (3)	−0.2346 (3)	0.0344 (7)	
O8	0.2897 (4)	0.3888 (3)	−0.0229 (2)	0.0336 (7)	
O9	0.5077 (4)	0.1801 (3)	−0.0249 (2)	0.0328 (6)	
O10	0.1025 (4)	0.4800 (3)	0.1838 (3)	0.0393 (7)	
O11	0.0268 (4)	−0.1150 (3)	−0.3466 (2)	0.0366 (7)	
O12	0.2504 (4)	0.3553 (4)	0.3249 (2)	0.0416 (8)	
N1	0.6350 (4)	0.4279 (3)	0.2668 (3)	0.0283 (7)	
H1A	0.7251	0.3830	0.2453	0.034*	
H1B	0.5404	0.3637	0.2389	0.034*	
C1	0.6718 (7)	0.4811 (5)	0.3856 (4)	0.0393 (10)	
H1C	0.6971	0.4019	0.4105	0.047*	
H1D	0.5712	0.5222	0.4090	0.047*	
C2	0.8249 (7)	0.5935 (5)	0.4315 (4)	0.0448 (11)	
H2A	0.8490	0.6295	0.5090	0.054*	
H2B	0.9264	0.5506	0.4106	0.054*	
C3	0.7596 (7)	0.6595 (5)	0.2798 (4)	0.0411 (11)	
H3A	0.8614	0.6180	0.2583	0.049*	
H3B	0.7394	0.7402	0.2561	0.049*	
C4	0.6052 (6)	0.5484 (5)	0.2269 (4)	0.0389 (10)	
H4A	0.5012	0.5912	0.2435	0.047*	
H4B	0.5895	0.5130	0.1499	0.047*	
C5	−0.2731 (15)	0.2565 (11)	−0.3890 (8)	0.054 (3)	0.50
H5A	−0.3428	0.2530	−0.3402	0.064*	0.50

H5B	−0.1983	0.3460	−0.3567	0.064*	0.50
C6	−0.1584 (11)	0.1245 (9)	−0.4092 (8)	0.040 (2)	0.50
H6A	−0.0830	0.1297	−0.4547	0.048*	0.50
H6B	−0.0875	0.1239	−0.3421	0.048*	0.50
C7	−0.468 (2)	0.1422 (11)	−0.5420 (8)	0.080 (5)	0.50
H7A	−0.5141	0.1491	−0.6114	0.095*	0.50
H7B	−0.5667	0.1395	−0.5115	0.095*	0.50
C8	−0.4008 (15)	−0.0005 (11)	−0.5624 (8)	0.048 (2)	0.50
H8A	−0.3368	−0.0183	−0.6174	0.057*	0.50
H8B	−0.4971	−0.0746	−0.5883	0.057*	0.50
N2	−0.2850 (10)	−0.0078 (8)	−0.4633 (6)	0.0391 (17)	0.50
H2C	−0.2270	−0.0865	−0.4799	0.047*	0.50
H2D	−0.3490	−0.0146	−0.4185	0.047*	0.50
O14	−0.3839 (10)	0.2508 (8)	−0.4885 (6)	0.0518 (19)	0.50
H5	0.671 (5)	0.141 (2)	−0.174 (3)	0.059 (18)*	
H4	0.563 (5)	0.015 (5)	−0.215 (4)	0.07 (2)*	
H8	0.853 (7)	0.376 (5)	0.881 (4)	0.054 (17)*	
H7	0.759 (8)	0.397 (4)	0.957 (4)	0.08 (2)*	
H1	−0.035 (5)	0.242 (5)	−0.021 (4)	0.045 (15)*	
H2	−0.173 (4)	−0.035 (4)	−0.183 (3)	0.031 (12)*	
H3	0.308 (5)	−0.055 (5)	−0.010 (4)	0.039 (14)*	
Cr1	0.0000	0.0000	0.0000	0.01611 (17)	
Mo1	0.30066 (4)	0.22031 (3)	−0.01793 (2)	0.02057 (11)	
Mo2	0.14776 (4)	−0.08727 (3)	−0.22125 (2)	0.02130 (11)	
Mo3	0.13429 (4)	0.31724 (3)	0.19717 (3)	0.02276 (11)	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0201 (12)	0.0182 (12)	0.0251 (13)	0.0049 (10)	0.0060 (10)	0.0102 (11)
O13	0.065 (2)	0.0260 (15)	0.0362 (17)	−0.0043 (15)	0.0085 (16)	0.0054 (13)
O2	0.0194 (12)	0.0202 (12)	0.0214 (13)	0.0032 (10)	0.0029 (10)	0.0079 (10)
O1W	0.051 (2)	0.0317 (16)	0.049 (2)	0.0146 (15)	0.0166 (16)	0.0209 (16)
O3	0.0171 (12)	0.0195 (12)	0.0259 (13)	0.0052 (10)	0.0059 (10)	0.0114 (10)
O2W	0.0327 (17)	0.043 (2)	0.061 (2)	0.0049 (15)	0.0136 (16)	0.0219 (19)
O4	0.0311 (14)	0.0210 (13)	0.0245 (13)	0.0018 (11)	0.0070 (11)	0.0107 (11)
O5	0.0199 (12)	0.0282 (14)	0.0225 (13)	−0.0010 (10)	0.0049 (10)	0.0065 (11)
O6	0.0253 (13)	0.0177 (12)	0.0335 (14)	0.0020 (10)	0.0123 (11)	0.0071 (11)
O7	0.0316 (15)	0.0301 (15)	0.0453 (17)	0.0041 (12)	0.0194 (13)	0.0121 (13)
O8	0.0441 (17)	0.0230 (14)	0.0371 (16)	0.0033 (12)	0.0132 (14)	0.0127 (12)
O9	0.0245 (14)	0.0360 (16)	0.0393 (16)	0.0023 (12)	0.0114 (12)	0.0129 (13)
O10	0.0471 (19)	0.0217 (14)	0.054 (2)	0.0064 (13)	0.0241 (16)	0.0113 (14)
O11	0.0443 (18)	0.0374 (17)	0.0263 (15)	0.0009 (14)	0.0069 (13)	0.0104 (13)
O12	0.0386 (17)	0.052 (2)	0.0251 (15)	−0.0105 (15)	0.0043 (13)	0.0051 (14)
N1	0.0234 (16)	0.0205 (16)	0.0365 (18)	0.0029 (12)	0.0053 (14)	0.0060 (14)
C1	0.052 (3)	0.034 (2)	0.038 (2)	0.003 (2)	0.015 (2)	0.017 (2)
C2	0.059 (3)	0.039 (3)	0.029 (2)	−0.003 (2)	0.001 (2)	0.010 (2)
C3	0.057 (3)	0.030 (2)	0.038 (2)	0.000 (2)	0.011 (2)	0.0153 (19)

C4	0.040 (2)	0.035 (2)	0.038 (2)	0.0034 (19)	0.0001 (19)	0.014 (2)
C5	0.058 (7)	0.037 (5)	0.040 (5)	−0.007 (5)	−0.005 (5)	−0.008 (4)
C6	0.029 (4)	0.025 (4)	0.060 (6)	−0.010 (3)	−0.023 (4)	0.029 (4)
C7	0.123 (11)	0.030 (5)	0.030 (5)	0.040 (6)	−0.042 (6)	−0.020 (4)
C8	0.062 (7)	0.040 (5)	0.031 (5)	0.007 (5)	0.003 (4)	0.005 (4)
N2	0.045 (4)	0.030 (4)	0.042 (4)	0.009 (3)	0.011 (3)	0.011 (3)
O14	0.060 (4)	0.048 (4)	0.072 (5)	0.026 (4)	0.021 (4)	0.048 (4)
Cr1	0.0156 (4)	0.0152 (4)	0.0185 (4)	0.0027 (3)	0.0045 (3)	0.0070 (3)
Mo1	0.02050 (17)	0.01772 (17)	0.02474 (18)	0.00128 (12)	0.00787 (12)	0.00772 (13)
Mo2	0.02274 (18)	0.02019 (18)	0.02183 (18)	0.00160 (12)	0.00814 (12)	0.00695 (13)
Mo3	0.02303 (18)	0.01904 (18)	0.02415 (18)	−0.00106 (12)	0.00799 (13)	0.00396 (13)

Geometric parameters (Å, º)

O1—Cr1	1.971 (2)	N1—H1B	0.9000
O1—Mo1	2.282 (2)	C1—C2	1.506 (7)
O1—Mo3	2.298 (3)	C1—H1C	0.9700
O1—H1	0.84 (1)	C1—H1D	0.9700
O13—C2	1.425 (6)	C2—H2A	0.9700
O13—C3	1.435 (5)	C2—H2B	0.9700
O2—Cr1	1.969 (2)	C3—C4	1.506 (6)
O2—Mo2	2.264 (3)	C3—H3A	0.9700
O2—Mo3^{i}	2.280 (3)	C3—H3B	0.9700
O2—H2	0.85 (1)	C4—H4A	0.9700
O1W—H8	0.85 (1)	C4—H4B	0.9700
O1W—H7	0.84 (1)	C5—O14	1.432 (12)
O3—Cr1	1.973 (2)	C5—C6	1.589 (14)
O3—Mo1	2.300 (2)	C5—H5A	0.9700
O3—Mo2	2.334 (3)	C5—H5B	0.9700
O3—H3	0.84 (1)	C6—N2	1.502 (10)
O2W—H5	0.85 (1)	C6—H6A	0.9700
O2W—H4	0.85 (1)	C6—H6B	0.9700
O4—Mo2	1.912 (3)	C7—O14	1.171 (13)
O4—Mo1	1.932 (3)	C7—C8	1.481 (13)
O5—Mo1	1.927 (3)	C7—H7A	0.9700
O5—Mo3	1.944 (3)	C7—H7B	0.9700
O6—Mo3	1.936 (3)	C8—N2	1.489 (12)
O6—Mo2^{i}	1.959 (3)	C8—H8A	0.9700
O7—Mo2	1.712 (3)	C8—H8B	0.9700
O8—Mo1	1.707 (3)	N2—H2C	0.9000
O9—Mo1	1.713 (3)	N2—H2D	0.9000
O10—Mo3	1.710 (3)	Cr1—O2^{i}	1.969 (2)
O11—Mo2	1.700 (3)	Cr1—O1^{i}	1.971 (2)
O12—Mo3	1.697 (3)	Cr1—O3^{i}	1.973 (2)
N1—C4	1.486 (5)	Mo2—O6^{i}	1.959 (3)
N1—C1	1.486 (5)	Mo3—O2^{i}	2.280 (3)
N1—H1A	0.9000		

Cr1—O1—Mo1	102.97 (10)	C7—C8—H8A	109.4
Cr1—O1—Mo3	102.58 (11)	N2—C8—H8A	109.4
Mo1—O1—Mo3	93.90 (9)	C7—C8—H8B	109.4
Cr1—O1—H1	123 (4)	N2—C8—H8B	109.4
Mo1—O1—H1	108 (4)	H8A—C8—H8B	108.0
Mo3—O1—H1	121 (4)	C8—N2—C6	109.9 (7)
C2—O13—C3	110.5 (3)	C8—N2—H2C	109.7
Cr1—O2—Mo2	103.98 (11)	C6—N2—H2C	109.7
Cr1—O2—Mo3^{i}	103.28 (11)	C8—N2—H2D	109.7
Mo2—O2—Mo3^{i}	94.50 (9)	C6—N2—H2D	109.7
Cr1—O2—H2	118 (3)	H2C—N2—H2D	108.2
Mo2—O2—H2	115 (3)	C7—O14—C5	117.2 (8)
Mo3^{i}—O2—H2	118 (3)	O2—Cr1—O2^{i}	180.00 (8)
H8—O1W—H7	109 (3)	O2—Cr1—O1	96.14 (11)
Cr1—O3—Mo1	102.31 (10)	O2^{i}—Cr1—O1	83.86 (11)
Cr1—O3—Mo2	101.36 (10)	O2—Cr1—O1^{i}	83.86 (11)
Mo1—O3—Mo2	91.99 (9)	O2^{i}—Cr1—O1^{i}	96.14 (11)
Cr1—O3—H3	123 (3)	O1—Cr1—O1^{i}	180.0 (2)
Mo1—O3—H3	117 (3)	O2—Cr1—O3^{i}	95.74 (11)
Mo2—O3—H3	115 (3)	O2^{i}—Cr1—O3^{i}	84.26 (11)
H5—O2W—H4	108 (2)	O1—Cr1—O3^{i}	95.80 (10)
Mo2—O4—Mo1	120.21 (13)	O1^{i}—Cr1—O3^{i}	84.20 (10)
Mo1—O5—Mo3	119.65 (13)	O2—Cr1—O3	84.26 (11)
Mo3—O6—Mo2^{i}	117.85 (13)	O2^{i}—Cr1—O3	95.74 (11)
C4—N1—C1	110.9 (3)	O1—Cr1—O3	84.20 (10)
C4—N1—H1A	109.4	O1^{i}—Cr1—O3	95.80 (10)
C1—N1—H1A	109.4	O3^{i}—Cr1—O3	180.00 (14)
C4—N1—H1B	109.4	O8—Mo1—O9	105.30 (14)
C1—N1—H1B	109.4	O8—Mo1—O5	100.53 (13)
H1A—N1—H1B	108.0	O9—Mo1—O5	97.80 (13)
N1—C1—C2	109.0 (4)	O8—Mo1—O4	96.53 (13)
N1—C1—H1C	109.9	O9—Mo1—O4	102.55 (13)
C2—C1—H1C	109.9	O5—Mo1—O4	148.89 (11)
N1—C1—H1D	109.9	O8—Mo1—O1	95.70 (12)
C2—C1—H1D	109.9	O9—Mo1—O1	157.96 (12)
H1C—C1—H1D	108.3	O5—Mo1—O1	71.37 (10)
O13—C2—C1	110.6 (4)	O4—Mo1—O1	81.24 (10)
O13—C2—H2A	109.5	O8—Mo1—O3	162.78 (12)
C1—C2—H2A	109.5	O9—Mo1—O3	89.88 (12)
O13—C2—H2B	109.5	O5—Mo1—O3	85.08 (10)
C1—C2—H2B	109.5	O4—Mo1—O3	71.79 (10)
H2A—C2—H2B	108.1	O1—Mo1—O3	70.48 (9)
O13—C3—C4	111.3 (4)	O11—Mo2—O7	105.69 (15)
O13—C3—H3A	109.4	O11—Mo2—O4	99.59 (13)
C4—C3—H3A	109.4	O7—Mo2—O4	100.91 (13)
O13—C3—H3B	109.4	O11—Mo2—O6^{i}	101.27 (13)
C4—C3—H3B	109.4	O7—Mo2—O6^{i}	94.73 (12)
H3A—C3—H3B	108.0	O4—Mo2—O6^{i}	149.40 (11)

N1—C4—C3	108.9 (4)	O11—Mo2—O2	91.86 (13)
N1—C4—H4A	109.9	O7—Mo2—O2	159.77 (12)
C3—C4—H4A	109.9	O4—Mo2—O2	85.64 (10)
N1—C4—H4B	109.9	O6^{i}—Mo2—O2	71.57 (10)
C3—C4—H4B	109.9	O11—Mo2—O3	160.09 (12)
H4A—C4—H4B	108.3	O7—Mo2—O3	93.59 (12)
O14—C5—C6	109.7 (8)	O4—Mo2—O3	71.32 (10)
O14—C5—H5A	109.7	O6^{i}—Mo2—O3	81.66 (10)
C6—C5—H5A	109.7	O2—Mo2—O3	70.19 (9)
O14—C5—H5B	109.7	O12—Mo3—O10	105.71 (17)
C6—C5—H5B	109.7	O12—Mo3—O6	101.54 (14)
H5A—C5—H5B	108.2	O10—Mo3—O6	97.65 (13)
N2—C6—C5	105.6 (7)	O12—Mo3—O5	95.12 (13)
N2—C6—H6A	110.6	O10—Mo3—O5	101.30 (13)
C5—C6—H6A	110.6	O6—Mo3—O5	150.28 (11)
N2—C6—H6B	110.6	O12—Mo3—O2^{i}	95.74 (14)
C5—C6—H6B	110.6	O10—Mo3—O2^{i}	157.68 (13)
H6A—C6—H6B	108.7	O6—Mo3—O2^{i}	71.59 (10)
O14—C7—C8	123.5 (11)	O5—Mo3—O2^{i}	82.47 (10)
O14—C7—H7A	106.5	O12—Mo3—O1	160.85 (13)
C8—C7—H7A	106.5	O10—Mo3—O1	90.09 (13)
O14—C7—H7B	106.5	O6—Mo3—O1	86.65 (10)
C8—C7—H7B	106.5	O5—Mo3—O1	70.75 (10)
H7A—C7—H7B	106.5	O2^{i}—Mo3—O1	70.22 (9)
C7—C8—N2	111.0 (7)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O6^{ii}	0.90	1.86	2.755 (4)	172
N1—H1*B*···O5	0.90	1.94	2.783 (4)	155
N2—H2*C*···O13^{iii}	0.90	2.19	2.976 (8)	145
N2—H2*D*···O2*W*^{iv}	0.90	2.53	3.294 (9)	144
O1—H1···O1*W*^{v}	0.84 (1)	1.87 (1)	2.709 (4)	173 (5)
O2—H2···O2*W*^{iv}	0.85 (1)	1.80 (1)	2.640 (4)	172 (4)
O3—H3···O9^{vi}	0.84 (1)	2.02 (1)	2.853 (4)	171 (5)
O1*W*—H7···O8^{vii}	0.84 (1)	2.08 (3)	2.837 (4)	148 (5)
O1*W*—H8···O10^{vii}	0.85 (1)	2.01 (2)	2.807 (5)	157 (5)
O2*W*—H4···O7	0.85 (1)	2.03 (2)	2.851 (4)	165 (5)
O2*W*—H5···O1*W*^{viii}	0.85 (1)	2.00 (2)	2.801 (5)	157 (4)

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