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Crystal structure of potassium sodium hepta-hydrogen hexamolybdocobaltate(III) octahydrate: an extra-protonated *B*-series Anderson-type heteropolyoxidometalate

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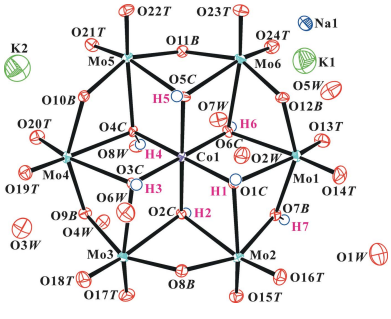
The title compound, $KNa[Co^{III}(OH)_7\{Mo_6O_{17}\}]\cdot 8H_2O$, was obtained by the ion-exchange technique from $K_3[Co(\mu_3\text{-}OH)_6Mo_6O_{18}]\cdot 7H_2O$. Six μ_3-O atoms and one O atom of the bridging μ_2-O atom are protonated. This novel polyanion protonated by an extra H atom is an unexpected polyanion species among the *B*-series Anderson-type polyoxidometalates (POMs), $[X^{n+}(\mu_3\text{-}OH)_6Mo_6O_{18}]^{(6-n)-}$ (X = heteroatom). The extra H atom (seventh H atom) in the polyanion does not lie on a crystallographic centre of symmetry, but is located at the mid-point between two μ_2-O atoms of adjacent polyanions, and forms a very short hydrogen bond [2.430 (5) Å]. The present structure is considered as particularly significant in understanding noncentrosymmetric strong hydrogen bonding.

1. Chemical context

The six H atoms attached to the μ_3-O atoms of the central $[XO_6]$ (X = heteroatom) octahedron in *B*-series Anderson-type heteropolyoxidomolybdates (Anderson, 1937; Tsigdinos, 1978), $[X^{n+}(\mu_3\text{-}OH)_6Mo_6O_{18}]^{(6-n)-}$ [X^{n+} = Ni^{2+} (Lee *et al.*, 2002), Cu^{2+} (Ito *et al.*, 1989), Al^{3+} (Lee *et al.*, 1991), Cr^{3+} (Perloff, 1970), Co^{3+} (Nolan *et al.*, 1998; Lee *et al.*, 2001), Rh^{3+} (Ozawa *et al.*, 1991)], are non-acidic (*i.e.* nondissociative). For the past four decades, the existence of a protonated species with more than seven H^+ ions was not expected for this class of compounds; the supposed highest number of seven was shown by $K_2[H_7Cr^{III}Mo_6O_{24}]\cdot 8H_2O$ (Joo *et al.*, 2015*a*). A free-acid type compound, $H_3[H_6AlMo_6O_{24}]\cdot 10H_2O$ (Liu *et al.*, 2006), was reported but the positions of protonated O atoms by the excess three H^+ ions were not defined. The current study was carried out to confirm the presence of a highly protonated species that exists at very low pH.

Considering the geometry of the interpolyanion hydrogen bonds by an extra H atom (seventh H atom), observed *via* electron-density maps around the protonated μ_2-O*B* atoms and bond valence sums (BVSs; Brown & Altermatt, 1985; Brese & O'Keeffe, 1991) of the protonated μ_2-O*B* atoms in the polyanion, we can determine that the positions of the extra H atoms follow a pseudosymmetric model in the polyanion. Sometimes a short hydrogen bond (O···O ⟨ 2.60 Å), in which the H atom lies on a crystallographic centre of symmetry, occurs in this class of structure (Lee *et al.*, 2010; Joo *et al.*, 2015*b*). The focus of this report is to clarify the position of the extra H atom of the polyanion in the title compound.



2. Structural commentary

Fig. 1 shows the the components of the crystal structure of the title compound. The O atoms of the heteropolyanion have been designated as O*T* (terminal Mo=O atom), O*B* (bridging μ_2-O*B* atom; Mo—O—Mo), and O*C* (centred μ_3-O atom; Mo_2—O*C*—Co). The protonated O atoms in the polyanion were confirmed by the BVSs, the charge balance, the bond-length elongation and the interpolyanion hydrogen bonds (Fig. 3 and Table 1).

Consider the symmetry relation of O7*B* and O10*B* atoms, the electron density of the H atom between atoms O7*B* and O10*B* in the difference Fourier map (Fig. 2) and the very short O7*B*···O10*B* distance of 2.430 (5) Å. Also consider the bond elongations by protonation of Mo1/2—O7*B* and Mo4/5—O10*B*, and the bond angles of Mo—O*B*—Mo. These data suggest that O7*B* or O10*B* in the polyanion should be protonated.

Confirmation of the protonated O atom was strongly supported by the BVS analysis. The calculated BVSs for expected protonation atoms O7*B* and O10*B* are 1.63 and 1.61 valence units (v.u.), respectively, if the valence of the O—H bond is not included. Since the BVS value around the O atom should be 2.0 v.u., the missing valences of O7*B* and O10*B* are 0.37 and 0.39 v.u., respectively, which corresponds to the valence of the O—H bonds. The BVS values for the unprotonated O8*B*, O9*B*, O11*B* and O12*B* atoms are 1.98, 1.94, 1.95 and 1.95 v.u., respectively. The reasonable BVSs of short and long O—H bond lengths can be obtained from the graphical correlation valences (Brown, 2002). This showed that atom H7 in the polyanion has a distance of 1.21 Å with 0.41 v.u. As a result, the valence sums around O7*B* and O10*B* are 2.04 and 2.01 v.u., respectively. Therefore, these valence unit values satisfy the protonation conditions of O7*B* and O10*B* atoms in the polyanion. As a result, these data suggest that H7 is located on the midpoint between O7*B* and O10*B*^{ii} atoms (the symmetry code corresponds to that in Fig. 3). However, the H7 atom contributes to the short hydrogen bonds, and does not lie on a crystallographic centre of symmetry; also, the electron density is not symmetric in the polyanion (Fig. 2), although we expect H7 atom to lie in the middle of the bond, which corresponds to a pseudosymmetric short hydrogen bond. This means that an extra H atom is co-shared by an adjacent polyanion; for example, μ_2-O7*B*···H7···μ_2-O10*B*^{ii} (Fig. 3).

The BVSs for the K1, K2, and Na1 ions are 0.50, 0.55, and 1.26 v.u, respectively, in the title compound (Na···O ⟨ 2.50 Å and K···O ⟨ 3.00 Å). BVS calculations for K1 and K2 reveal a considerable under-saturation in terms of valence units, which we ascribe to the disordered character of the K^+ position. All

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*C*—H1···O2*W*	0.85 (3)	1.81 (3)	2.639 (6)	167 (7)
O2*C*—H2···O22*T*^{i}	0.81 (3)	1.98 (3)	2.787 (6)	170 (7)
O3*C*—H3···O6*W*	0.84 (3)	1.99 (4)	2.775 (6)	154 (6)
O4*C*—H4···O8*W*	0.84 (3)	1.81 (3)	2.627 (6)	165 (7)
O5*C*—H5···O15*T*^{ii}	0.83 (3)	1.99 (3)	2.822 (6)	171 (7)
O6*C*—H6···O7*W*	0.82 (3)	1.96 (3)	2.761 (6)	165 (7)
O7*B*—H7···O10*B*^{i}	1.21 (2)	1.22 (2)	2.430 (5)	175 (6)
O1*W*—H1*B*···O14*T*	0.86 (3)	1.89 (4)	2.731 (7)	163 (8)
O1*W*—H1*A*···O16*T*	0.85 (3)	2.18 (5)	2.878 (7)	140 (6)
O2*W*—H2*A*···O8*W*^{iii}	0.85 (3)	1.91 (3)	2.757 (6)	176 (7)
O2*W*—H2*B*···O15*T*^{ii}	0.83 (3)	2.13 (4)	2.841 (6)	145 (6)
O3*W*—H3*B*···O19*T*	0.83 (3)	2.01 (3)	2.792 (7)	156 (6)
O3*W*—H3*A*···O1*W*^{ii}	0.83 (3)	2.02 (4)	2.784 (7)	154 (8)
O4*W*—H4*A*···O23*T*^{i}	0.84 (3)	1.97 (3)	2.800 (6)	167 (7)
O4*W*—H4*B*···O9*B*	0.84 (3)	1.91 (3)	2.734 (6)	167 (7)
O6*W*—H6*B*···O3*W*	0.84 (3)	1.88 (3)	2.709 (7)	169 (7)
O6*W*—H6*A*···O11*B*^{iii}	0.83 (3)	2.31 (6)	2.921 (6)	131 (6)
O7*W*—H7*A*···O8*B*^{iv}	0.81 (3)	2.42 (6)	2.937 (6)	122 (6)
O7*W*—H7*B*···O6*W*^{iv}	0.82 (3)	2.00 (3)	2.811 (7)	166 (8)
O8*W*—H8*B*···O4*W*	0.83 (3)	1.88 (3)	2.697 (7)	168 (7)
O8*W*—H8*A*···O7*W*	0.82 (3)	2.01 (4)	2.761 (8)	151 (7)

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

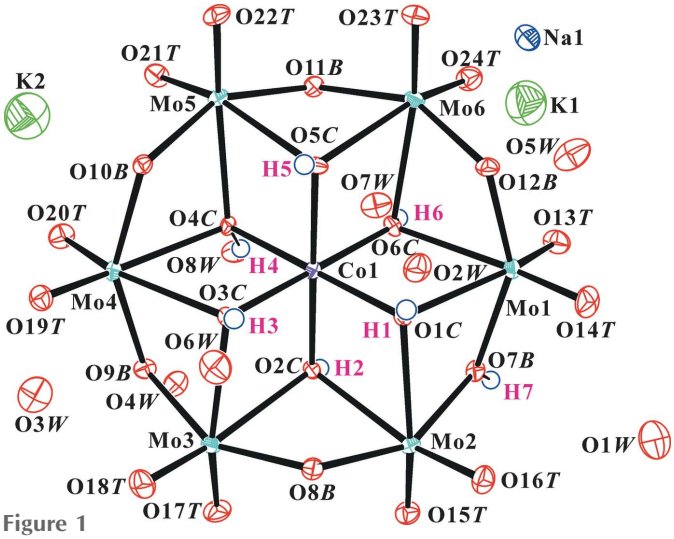


Figure 1
The polyanion structure and the cations as well as the lattice water molecules in the title compound. Displacement ellipsoids are drawn at the 50% probability level for non-H atoms. H atoms are drawn as small spheres of arbitrary radius.

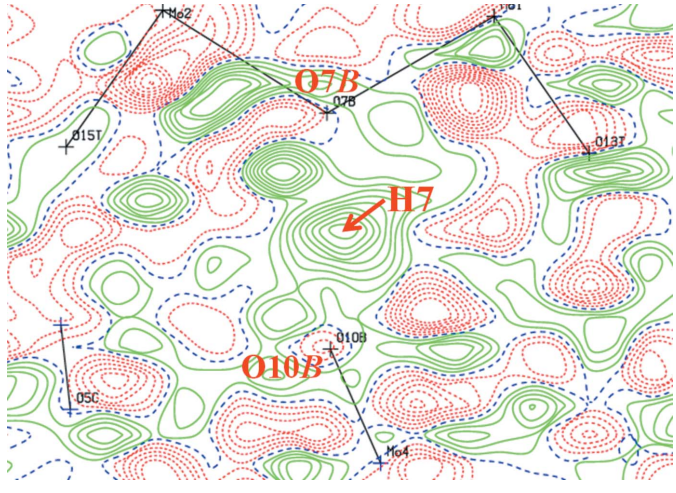


Figure 2
Difference Fourier map between atoms O7*B* and O10*B*, where H atoms were absent.

Table 2
Experimental details.

Crystal data	
Chemical formula	$KNa[CoMo_6O_{17}(OH)_7]\cdot 8H_2O$
M_r	1231.84
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	173
a, b, c (Å)	10.9758 (5), 20.7702 (9), 12.7906 (6)
β (°)	99.666 (1)
V (Å^3)	2874.5 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.37
Crystal size (mm)	0.20 × 0.10 × 0.05
Data collection	
Diffractometer	Bruker SMART APEXII CCD diffractometer
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.669, 0.838
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17925, 6701, 4416
R_{int}	0.043
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.666
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.081, 1.06
No. of reflections	6701
No. of parameters	449
No. of restraints	31
H-atom treatment	Only H-atom coordinates refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.02, −1.06

Computer programs: *APEX2* (Bruker, 2009), *SAINT* (Bruker, 2009), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *PLATON* (Spek, 2009) and *DIAMOND* (Brandenburg, 1998).

the BVSs agree well with the charge-balance requirements. The K^+ ions are coordinated by four and three O atoms as $[K1(OW)(OB)(OT)_2]^+$ and $[K2(OW)_2(OT)_2]^+$. The Na^+ ion is coordinated by six O atoms as $[Na1(OW)_4(OT)_2]^+$.

3. Supramolecular features

The polyanions are linked together into chains along [101] *via* hydrogen bonds: two normal inter-polyanion μ_3-O (O*C*)···μ_1-O (O*T*) and one very short μ_2-O7*B*–H7···μ_2-O10*B* bond (Fig. 3 and Table 1). Note that water molecules O6*W*, O7*W* and O8*W* do not show any interaction with the metal atoms and are bonded to other O atoms only by hydrogen bonds. The other H atoms of the polyanion, (H1, H3, H4 and H6) form hydrogen bonds with water molecules (Table 1).

4. Synthesis and crystallization

Title compound was obtained from the ion-exchanged solution (*ca* pH 1.4) of $K_3[H_6CoMo_6O_{24}]\cdot 7H_2O$ (Lee *et al.*, 2001) by Amberlite IR120. The resulting solution was concentrated in a hot water bath. After 1 d, stable blue crystals were obtained at room temperature. The Na^+ ion in the title compound is considered to have been a contaminant from the ion-exchange resin.

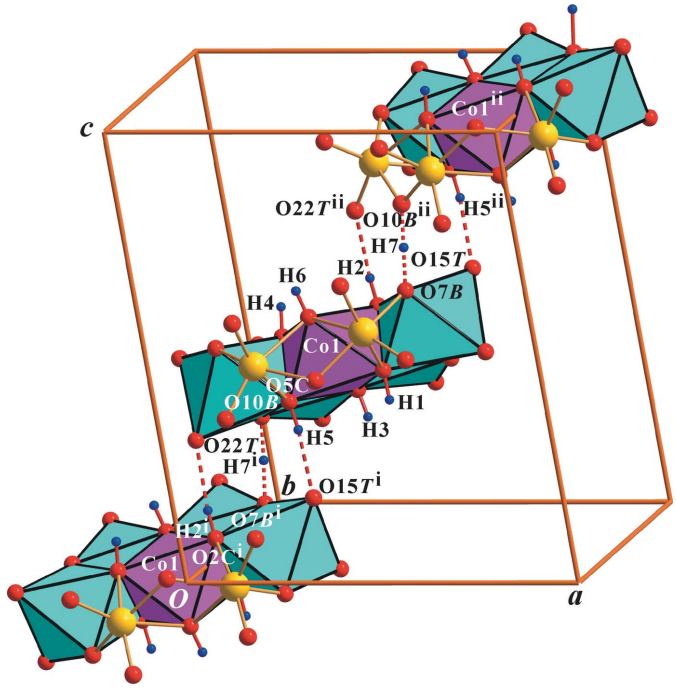


Figure 3
Polyhedral view with unit cell of the heteropolyanion in the title compound, with the O···O contacts of the interpolyanion hydrogen bonds shown as dashed lines. [Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.]

5. Refinement

The crystal data, the data collection and the structure refinement details are summarized in Table 2. All H atoms in the polyanion and all H atoms in the water molecules were located from difference Fourier maps. All H atoms of the polyanion were refined with a distance restraint of O—H = 0.85 (3) Å, except O7*B*–H7, and were included in the refinement with U_{iso}(H) = 1.5U_{eq}(O). The bond lengths of O7*B*—H7 and O10*B*—H7^i (the symmetry code corresponds to that in Fig. 3) were constrained by using the SADI (σ = 0.03) command; they were set to be equal with an effective standard uncertainty to locate the shared H atom on the pseudocentre between atoms O7*B* and O10*B*. The H atoms of all the water molecules (O*W*) were refined with distances and angles restraints of O—H = 0.85 (3) Å and H*A*···H*B* = 1.35 (3) Å, and were included in the refinement with U_{iso}(H) = 1.5U_{eq}(O). Reasonable displacement ellipsoids of K1 and K2 were obtained with half-occupancy.

Acknowledgements

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Crystal structure of potassium sodium heptahydrogen hexamolybdocobaltate(III) octahydrate: an extra-protonated *B*-series Anderson-type heteropolyoxidometalate

Ki-Min Park, Hea-Chung Joo and Uk Lee

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012), *PLATON* (Spek, 2009) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXL2014* (Sheldrick, 2015).

Sodium potassium hexa-μ_3-hydroxido-μ_2-hydroxido-heptadecaoxidocobaltate(II)hexamolybdate(VI) octahydrate

Crystal data

$KNa[CoMo_6O_{17}(OH)_7]\cdot 8H_2O$
M_r = 1231.84
Monoclinic, $P2_1/n$
a = 10.9758 (5) Å
b = 20.7702 (9) Å
c = 12.7906 (6) Å
β = 99.666 (1)°
V = 2874.5 (2) Å^3
Z = 4
$F(000)$ = 2352
D_x = 2.846 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5031 reflections
θ = 2.5–28.2°
μ = 3.37 mm^{-1}
T = 173 K
Block, blue
0.20 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: rotating anode
Detector resolution: 10.0 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.669, T_{max} = 0.838
17925 measured reflections
6701 independent reflections
4416 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 28.3°, θ_{min} = 1.9°
h = −14→14
k = −27→10
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.081
S = 1.06
6701 reflections
449 parameters
31 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
Only H-atom coordinates refined
$w = 1/[\sigma^2(F_o^2) + (0.0192P)^2 + 12.1333P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.02 e Å^{-3}
$\Delta\rho_{min}$ = −1.06 e Å^{-3}

Extinction correction: *SHELXL2014* (Sheldrick, 2015), $Fc^{*}=kFc[1+0.001xFc^{2}\lambda^{3}/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00011 (2)

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_{iso}*/U_{eq}	Occ. (<1)
Mo1	0.53782 (5)	0.10915 (3)	0.53624 (4)	0.01162 (13)	
Mo2	0.71702 (5)	0.24276 (3)	0.53614 (4)	0.01042 (12)	
Mo3	0.58803 (5)	0.38359 (3)	0.47083 (4)	0.01109 (12)	
Mo4	0.28516 (5)	0.39351 (3)	0.39378 (4)	0.01036 (12)	
Mo5	0.10877 (5)	0.25896 (3)	0.38934 (4)	0.01082 (12)	
Mo6	0.23869 (5)	0.11899 (3)	0.45827 (4)	0.01178 (13)	
Co1	0.41250 (8)	0.25144 (4)	0.46414 (7)	0.00890 (16)	
K1	0.3893 (4)	0.0424 (2)	0.2202 (3)	0.0427 (10)	0.5
K2	−0.0640 (5)	0.4290 (3)	0.5040 (4)	0.0659 (14)	0.5
Na1	0.1547 (3)	0.01011 (12)	0.7104 (2)	0.0225 (6)	
O1C	0.5469 (4)	0.1996 (2)	0.4361 (3)	0.0099 (9)	
H1	0.552 (6)	0.192 (3)	0.372 (3)	0.015*	
O2C	0.5375 (4)	0.2937 (2)	0.5617 (3)	0.0093 (9)	
H2	0.530 (6)	0.292 (3)	0.624 (3)	0.014*	
O3C	0.4390 (4)	0.3205 (2)	0.3718 (3)	0.0086 (9)	
H3	0.455 (6)	0.310 (3)	0.312 (3)	0.013*	
O4C	0.2764 (4)	0.3033 (2)	0.4915 (3)	0.0093 (9)	
H4	0.285 (6)	0.307 (3)	0.557 (2)	0.014*	
O5C	0.2891 (4)	0.2085 (2)	0.3653 (3)	0.0108 (9)	
H5	0.299 (6)	0.210 (3)	0.302 (3)	0.016*	
O6C	0.3851 (4)	0.1826 (2)	0.5565 (3)	0.0108 (9)	
H6	0.365 (6)	0.181 (3)	0.615 (3)	0.016*	
O7B	0.6477 (4)	0.1741 (2)	0.6169 (3)	0.0111 (9)	
H7	0.664 (6)	0.171 (3)	0.7129 (13)	0.017*	
O8B	0.6943 (4)	0.3130 (2)	0.4423 (3)	0.0125 (9)	
O9B	0.4270 (4)	0.4140 (2)	0.4939 (3)	0.0120 (9)	
O10B	0.1788 (4)	0.3281 (2)	0.3095 (3)	0.0109 (9)	
O11B	0.1319 (4)	0.1898 (2)	0.4860 (3)	0.0117 (9)	
O12B	0.3973 (4)	0.0895 (2)	0.4323 (3)	0.0127 (9)	
O13T	0.5124 (4)	0.0676 (2)	0.6458 (4)	0.0198 (11)	
O14T	0.6444 (4)	0.0669 (2)	0.4824 (4)	0.0210 (11)	
O15T	0.8019 (4)	0.2762 (2)	0.6482 (3)	0.0162 (10)	
O16T	0.8163 (4)	0.1981 (2)	0.4768 (3)	0.0176 (10)	
O17T	0.6726 (4)	0.4151 (2)	0.5825 (3)	0.0194 (11)	
O18T	0.6115 (4)	0.4313 (2)	0.3682 (3)	0.0191 (11)	
O19T	0.3029 (4)	0.4388 (2)	0.2856 (3)	0.0152 (10)	

O20T	0.1757 (4)	0.4314 (2)	0.4505 (3)	0.0179 (10)
O21T	0.0045 (4)	0.3034 (2)	0.4433 (3)	0.0158 (10)
O22T	0.0288 (4)	0.2243 (2)	0.2763 (3)	0.0152 (10)
O23T	0.1523 (4)	0.0867 (2)	0.3471 (3)	0.0185 (10)
O24T	0.2177 (4)	0.0719 (2)	0.5621 (4)	0.0195 (11)
O1W	0.8736 (5)	0.0678 (3)	0.4260 (4)	0.0275 (12)
H1A	0.889 (6)	0.1078 (16)	0.427 (6)	0.041*
H1B	0.796 (3)	0.067 (3)	0.430 (6)	0.041*
O2W	0.5288 (4)	0.1640 (2)	0.2360 (4)	0.0182 (10)
H2A	0.601 (3)	0.169 (3)	0.223 (5)	0.027*
H2B	0.484 (5)	0.187 (3)	0.193 (5)	0.027*
O3W	0.4675 (4)	0.4437 (3)	0.1413 (4)	0.0241 (11)
H3A	0.450 (6)	0.452 (4)	0.077 (2)	0.036*
H3B	0.403 (4)	0.445 (4)	0.168 (5)	0.036*
O4W	0.4278 (4)	0.4240 (2)	0.7072 (3)	0.0184 (10)
H4A	0.497 (4)	0.416 (4)	0.744 (4)	0.028*
H4B	0.436 (6)	0.426 (4)	0.643 (2)	0.028*
O5W	0.3599 (5)	0.0204 (3)	0.7925 (4)	0.0372 (14)
H5A	0.391 (8)	0.048 (3)	0.757 (5)	0.056*
H5B	0.385 (8)	0.029 (4)	0.857 (2)	0.056*
O6W	0.5384 (5)	0.3204 (2)	0.1861 (4)	0.0217 (11)
H6A	0.526 (7)	0.303 (3)	0.127 (3)	0.033*
H6B	0.526 (7)	0.3600 (14)	0.176 (5)	0.033*
O7W	0.2948 (4)	0.1969 (3)	0.7441 (4)	0.0247 (12)
H7A	0.322 (6)	0.188 (4)	0.805 (3)	0.037*
H7B	0.222 (3)	0.185 (4)	0.730 (5)	0.037*
O8W	0.2654 (4)	0.3256 (2)	0.6919 (3)	0.0193 (11)
H8A	0.284 (6)	0.293 (2)	0.728 (5)	0.029*
H8B	0.319 (5)	0.354 (2)	0.705 (5)	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.0123 (3)	0.0096 (3)	0.0125 (3)	0.0008 (2)	0.0008 (2)	0.0011 (2)
Mo2	0.0084 (2)	0.0118 (3)	0.0107 (3)	−0.0002 (2)	0.0006 (2)	0.0000 (2)
Mo3	0.0110 (2)	0.0106 (3)	0.0112 (3)	−0.0017 (2)	0.0005 (2)	0.0006 (2)
Mo4	0.0111 (2)	0.0097 (3)	0.0103 (3)	0.0016 (2)	0.0018 (2)	0.0003 (2)
Mo5	0.0089 (2)	0.0133 (3)	0.0098 (3)	−0.0002 (2)	0.0002 (2)	−0.0002 (2)
Mo6	0.0117 (3)	0.0112 (3)	0.0119 (3)	−0.0029 (2)	0.0004 (2)	0.0016 (2)
Co1	0.0090 (3)	0.0093 (4)	0.0084 (3)	0.0008 (3)	0.0013 (3)	0.0002 (3)
K1	0.045 (2)	0.038 (2)	0.044 (2)	0.0036 (19)	0.0044 (18)	−0.0032 (18)
K2	0.063 (3)	0.068 (4)	0.070 (3)	0.007 (3)	0.021 (3)	−0.006 (3)
Na1	0.0272 (14)	0.0186 (14)	0.0212 (13)	−0.0012 (13)	0.0029 (11)	−0.0004 (13)
O1C	0.011 (2)	0.009 (2)	0.010 (2)	−0.0001 (18)	0.0010 (18)	−0.0016 (18)
O2C	0.011 (2)	0.008 (2)	0.008 (2)	−0.0004 (17)	−0.0007 (18)	0.0012 (18)
O3C	0.013 (2)	0.009 (2)	0.004 (2)	−0.0002 (18)	0.0027 (17)	−0.0003 (17)
O4C	0.010 (2)	0.009 (2)	0.009 (2)	0.0023 (17)	0.0029 (18)	−0.0010 (18)
O5C	0.010 (2)	0.016 (2)	0.006 (2)	−0.0056 (18)	0.0015 (18)	−0.0016 (18)

O6C	0.014 (2)	0.010 (2)	0.008 (2)	−0.0010 (18)	0.0041 (18)	0.0010 (18)
O7B	0.013 (2)	0.013 (2)	0.006 (2)	0.0014 (18)	−0.0027 (17)	−0.0005 (17)
O8B	0.011 (2)	0.014 (2)	0.014 (2)	0.0002 (18)	0.0057 (18)	0.0032 (18)
O9B	0.012 (2)	0.013 (2)	0.010 (2)	−0.0009 (18)	0.0009 (17)	−0.0053 (18)
O10B	0.012 (2)	0.011 (2)	0.009 (2)	0.0002 (18)	−0.0007 (17)	0.0010 (17)
O11B	0.011 (2)	0.013 (2)	0.013 (2)	0.0011 (18)	0.0051 (18)	0.0001 (18)
O12B	0.011 (2)	0.014 (2)	0.012 (2)	−0.0031 (18)	−0.0013 (18)	−0.0013 (18)
O13T	0.021 (3)	0.019 (3)	0.018 (2)	−0.004 (2)	−0.001 (2)	0.006 (2)
O14T	0.020 (2)	0.020 (3)	0.023 (3)	0.007 (2)	0.006 (2)	−0.007 (2)
O15T	0.015 (2)	0.019 (3)	0.013 (2)	−0.002 (2)	−0.0006 (19)	0.0007 (19)
O16T	0.017 (2)	0.015 (3)	0.021 (2)	0.005 (2)	0.006 (2)	0.001 (2)
O17T	0.015 (2)	0.023 (3)	0.018 (2)	−0.002 (2)	−0.0047 (19)	−0.003 (2)
O18T	0.024 (3)	0.018 (3)	0.017 (2)	0.000 (2)	0.006 (2)	0.007 (2)
O19T	0.016 (2)	0.015 (2)	0.014 (2)	−0.0007 (18)	0.003 (2)	0.0028 (19)
O20T	0.016 (2)	0.020 (3)	0.018 (2)	0.002 (2)	0.0050 (19)	−0.002 (2)
O21T	0.014 (2)	0.016 (2)	0.019 (2)	−0.0010 (19)	0.0082 (19)	−0.003 (2)
O22T	0.013 (2)	0.020 (3)	0.012 (2)	−0.0023 (19)	−0.0017 (18)	0.0009 (19)
O23T	0.016 (2)	0.017 (3)	0.021 (2)	−0.005 (2)	−0.001 (2)	−0.004 (2)
O24T	0.018 (2)	0.021 (3)	0.019 (2)	−0.002 (2)	0.003 (2)	0.003 (2)
O1W	0.036 (3)	0.024 (3)	0.023 (3)	0.003 (3)	0.007 (2)	−0.004 (2)
O2W	0.015 (2)	0.021 (3)	0.020 (3)	0.002 (2)	0.005 (2)	−0.003 (2)
O3W	0.025 (3)	0.031 (3)	0.018 (2)	0.003 (2)	0.009 (2)	0.001 (2)
O4W	0.021 (2)	0.022 (3)	0.012 (2)	0.005 (2)	0.0032 (19)	−0.002 (2)
O5W	0.029 (3)	0.057 (4)	0.025 (3)	0.002 (3)	0.003 (3)	0.015 (3)
O6W	0.030 (3)	0.018 (3)	0.019 (2)	−0.002 (2)	0.008 (2)	0.001 (2)
O7W	0.021 (3)	0.038 (3)	0.016 (3)	−0.003 (2)	0.007 (2)	0.002 (2)
O8W	0.020 (2)	0.024 (3)	0.013 (2)	−0.006 (2)	0.003 (2)	−0.004 (2)

Geometric parameters (Å, º)

Mo1—O7B	1.980 (4)	K1—O5W^{ii}	3.076 (7)
Mo1—O12B	1.904 (4)	K1—O20T^{iv}	3.173 (6)
Mo2—O7B	1.985 (4)	K1—O23T	3.415 (6)
Mo2—O8B	1.879 (4)	K1—Mo4^{iv}	3.797 (4)
Mo3—O8B	1.946 (4)	K2—O20T	2.828 (6)
Mo3—O9B	1.946 (4)	K2—O21T	2.858 (7)
Mo4—O9B	1.892 (4)	K2—O5W^{i}	2.893 (8)
Mo4—O10B	1.987 (4)	K2—O17T^{v}	3.229 (7)
Mo5—O10B	1.990 (4)	K2—O20T^{vi}	3.237 (7)
Mo5—O11B	1.885 (4)	K2—Mo3^{v}	3.888 (5)
Mo6—O11B	1.950 (4)	Na1—O3W^{vii}	2.306 (6)
Mo6—O12B	1.927 (4)	Na1—O5W	2.329 (6)
Mo1—O14T	1.698 (4)	Na1—O4W^{viii}	2.335 (5)
Mo1—O13T	1.708 (5)	Na1—O1W^{ii}	2.361 (6)
Mo1—O1C	2.285 (4)	Na1—O18T^{vii}	2.471 (5)
Mo1—O6C	2.314 (4)	Na1—O24T	2.483 (5)
Mo2—O16T	1.703 (4)	Na1—H5A	2.68 (7)
Mo2—O15T	1.719 (4)	O1C—H1	0.85 (3)

Mo2—O1C	2.264 (4)	O2C—H2	0.81 (3)
Mo2—O2C	2.308 (4)	O3C—H3	0.84 (3)
Mo3—O18T	1.698 (4)	O4C—H4	0.84 (3)
Mo3—O17T	1.698 (4)	O5C—H5	0.83 (3)
Mo3—O3C	2.302 (4)	O6C—H6	0.82 (3)
Mo3—O2C	2.316 (4)	O7B—O10B^{ix}	2.430 (5)
Mo4—O20T	1.698 (4)	O7B—H7	1.213 (16)
Mo4—O19T	1.712 (4)	O13T—K1^{ii}	2.950 (6)
Mo4—O4C	2.264 (4)	O17T—K1^{ix}	2.852 (6)
Mo4—O3C	2.321 (4)	O17T—K2^{x}	3.228 (7)
Mo5—O21T	1.704 (4)	O18T—Na1^{iii}	2.471 (5)
Mo5—O22T	1.718 (4)	O19T—K1^{xi}	3.006 (6)
Mo5—O4C	2.266 (4)	O20T—K1^{xi}	3.172 (6)
Mo5—O5C	2.305 (4)	O20T—K2^{vi}	3.237 (7)
Mo6—O24T	1.696 (5)	O1W—H1A	0.85 (3)
Mo6—O23T	1.708 (4)	O1W—H1B	0.86 (3)
Mo6—O6C	2.287 (4)	O2W—H2A	0.85 (3)
Mo6—O5C	2.324 (4)	O2W—H2B	0.83 (3)
Co1—O2C	1.906 (4)	O3W—H3A	0.83 (3)
Co1—O1C	1.908 (4)	O3W—H3B	0.83 (3)
Co1—O6C	1.910 (4)	O4W—H4A	0.84 (3)
Co1—O5C	1.911 (4)	O4W—H4B	0.84 (3)
Co1—O3C	1.911 (4)	O5W—H5A	0.84 (3)
Co1—O4C	1.920 (4)	O5W—H5B	0.85 (3)
K1—O17T^{i}	2.852 (6)	O6W—H6A	0.83 (3)
K1—O12B	2.871 (6)	O6W—H6B	0.84 (3)
K1—O2W	2.943 (6)	O7W—H7A	0.81 (3)
K1—O13T^{ii}	2.950 (6)	O7W—H7B	0.82 (3)
K1—K2^{iii}	2.956 (6)	O8W—H8A	0.82 (3)
K1—O19T^{iv}	3.006 (6)	O8W—H8B	0.83 (3)

Mo1—O7B—Mo2	118.12 (19)	O1C—Co1—O6C	84.32 (18)
Mo2—O8B—Mo3	119.0 (2)	O2C—Co1—O5C	179.2 (2)
Mo4—O9B—Mo3	119.3 (2)	O1C—Co1—O5C	95.56 (18)
Mo4—O10B—Mo5	117.23 (19)	O6C—Co1—O5C	83.83 (18)
Mo5—O11B—Mo6	118.3 (2)	O2C—Co1—O3C	83.78 (17)
Mo1—O12B—Mo6	117.4 (2)	O1C—Co1—O3C	96.02 (18)
O14T—Mo1—O13T	106.9 (2)	O6C—Co1—O3C	179.6 (2)
O14T—Mo1—O12B	98.0 (2)	O5C—Co1—O3C	96.07 (17)
O13T—Mo1—O12B	103.87 (19)	O2C—Co1—O4C	96.82 (18)
O14T—Mo1—O7B	99.3 (2)	O1C—Co1—O4C	179.5 (2)
O13T—Mo1—O7B	94.91 (19)	O6C—Co1—O4C	95.66 (18)
O12B—Mo1—O7B	149.46 (18)	O5C—Co1—O4C	83.99 (18)
O14T—Mo1—O1C	95.71 (19)	O3C—Co1—O4C	83.99 (18)
O13T—Mo1—O1C	154.61 (19)	O17T^{i}—K1—O12B	111.63 (18)
O12B—Mo1—O1C	83.77 (16)	O17T^{i}—K1—O2W	98.47 (17)
O7B—Mo1—O1C	69.63 (15)	O12B—K1—O2W	73.14 (15)
O14T—Mo1—O6C	161.41 (19)	O17T^{i}—K1—O13T^{ii}	141.7 (2)

O13T—Mo1—O6C	91.12 (19)	O12B—K1—O13T^{ii}	76.40 (16)
O12B—Mo1—O6C	72.70 (16)	O2W—K1—O13T^{ii}	119.31 (18)
O7B—Mo1—O6C	83.21 (16)	O17T^{i}—K1—O19T^{iv}	72.37 (15)
O1C—Mo1—O6C	67.73 (15)	O12B—K1—O19T^{iv}	100.20 (17)
O16T—Mo2—O15T	107.1 (2)	O2W—K1—O19T^{iv}	166.19 (19)
O16T—Mo2—O8B	99.4 (2)	O13T^{ii}—K1—O19T^{iv}	69.30 (14)
O15T—Mo2—O8B	102.4 (2)	K2^{iii}—K1—O19T^{iv}	110.61 (18)
O16T—Mo2—O7B	99.8 (2)	O17T^{i}—K1—O5W^{ii}	139.4 (2)
O15T—Mo2—O7B	93.30 (18)	O12B—K1—O5W^{ii}	107.96 (17)
O8B—Mo2—O7B	150.30 (17)	O2W—K1—O5W^{ii}	84.68 (18)
O16T—Mo2—O1C	93.51 (18)	O13T^{ii}—K1—O5W^{ii}	57.22 (15)
O15T—Mo2—O1C	155.67 (18)	K2^{iii}—K1—O5W^{ii}	74.83 (17)
O8B—Mo2—O1C	86.44 (16)	O19T^{iv}—K1—O5W^{ii}	109.03 (18)
O7B—Mo2—O1C	70.01 (15)	O17T^{i}—K1—O20T^{iv}	74.43 (15)
O16T—Mo2—O2C	159.74 (18)	O12B—K1—O20T^{iv}	149.92 (19)
O15T—Mo2—O2C	93.03 (17)	O2W—K1—O20T^{iv}	136.46 (19)
O8B—Mo2—O2C	73.14 (16)	O13T^{ii}—K1—O20T^{iv}	81.66 (16)
O7B—Mo2—O2C	81.06 (16)	K2^{iii}—K1—O20T^{iv}	63.66 (15)
O1C—Mo2—O2C	67.59 (15)	O19T^{iv}—K1—O20T^{iv}	52.21 (13)
O18T—Mo3—O17T	107.0 (2)	O5W^{ii}—K1—O20T^{iv}	75.85 (16)
O18T—Mo3—O9B	100.8 (2)	O17T^{i}—K1—O23T	65.64 (14)
O17T—Mo3—O9B	97.41 (19)	O12B—K1—O23T	50.53 (12)
O18T—Mo3—O8B	97.0 (2)	O2W—K1—O23T	99.51 (16)
O17T—Mo3—O8B	100.8 (2)	O13T^{ii}—K1—O23T	99.58 (16)
O9B—Mo3—O8B	149.52 (18)	K2^{iii}—K1—O23T	130.99 (18)
O18T—Mo3—O3C	95.35 (18)	O19T^{iv}—K1—O23T	67.49 (14)
O17T—Mo3—O3C	156.84 (19)	O5W^{ii}—K1—O23T	154.08 (18)
O9B—Mo3—O3C	71.88 (15)	O20T^{iv}—K1—O23T	114.93 (16)
O8B—Mo3—O3C	82.01 (16)	O20T—K2—O17T^{v}	174.2 (2)
O18T—Mo3—O2C	159.84 (19)	O21T—K2—O17T^{v}	107.0 (2)
O17T—Mo3—O2C	91.83 (18)	O5W^{i}—K2—O17T^{v}	101.0 (2)
O9B—Mo3—O2C	83.43 (16)	K1^{vii}—K2—O17T^{v}	54.70 (13)
O8B—Mo3—O2C	71.85 (16)	O20T—K2—O20T^{vi}	115.0 (2)
O3C—Mo3—O2C	67.00 (14)	O21T—K2—O20T^{vi}	172.2 (2)
O20T—Mo4—O19T	106.0 (2)	O5W^{i}—K2—O20T^{vi}	77.54 (19)
O20T—Mo4—O9B	99.62 (19)	K1^{vii}—K2—O20T^{vi}	61.43 (14)
O19T—Mo4—O9B	103.35 (19)	O17T^{v}—K2—O20T^{vi}	68.79 (15)
O20T—Mo4—O10B	98.97 (19)	O3W^{vii}—Na1—O5W	150.1 (2)
O19T—Mo4—O10B	94.22 (18)	O3W^{vii}—Na1—O4W^{viii}	95.9 (2)
O9B—Mo4—O10B	149.70 (18)	O5W—Na1—O4W^{viii}	106.6 (2)
O20T—Mo4—O4C	92.86 (19)	O3W^{vii}—Na1—O1W^{ii}	90.2 (2)
O19T—Mo4—O4C	157.33 (18)	O5W—Na1—O1W^{ii}	113.2 (2)
O9B—Mo4—O4C	85.36 (17)	O4W^{viii}—Na1—O1W^{ii}	78.19 (19)
O10B—Mo4—O4C	69.99 (15)	O3W^{vii}—Na1—O18T^{vii}	80.04 (18)
O20T—Mo4—O3C	159.40 (18)	O5W—Na1—O18T^{vii}	83.7 (2)
O19T—Mo4—O3C	94.43 (17)	O4W^{viii}—Na1—O18T^{vii}	82.32 (18)
O9B—Mo4—O3C	72.33 (16)	O1W^{ii}—Na1—O18T^{vii}	157.2 (2)
O10B—Mo4—O3C	81.98 (15)	O3W^{vii}—Na1—O24T	80.59 (18)

O4C—Mo4—O3C	67.98 (15)	O5W—Na1—O24T	85.70 (19)
O21T—Mo5—O22T	106.6 (2)	O4W^{viii}—Na1—O24T	156.9 (2)
O21T—Mo5—O11B	99.98 (19)	O1W^{ii}—Na1—O24T	78.99 (19)
O22T—Mo5—O11B	103.08 (19)	O18T^{vii}—Na1—O24T	119.07 (18)
O21T—Mo5—O10B	99.22 (19)	Co1—O1C—Mo2	105.09 (18)
O22T—Mo5—O10B	93.26 (18)	Co1—O1C—Mo1	104.52 (18)
O11B—Mo5—O10B	149.96 (17)	Mo2—O1C—Mo1	96.78 (15)
O21T—Mo5—O4C	94.70 (18)	Co1—O2C—Mo2	103.52 (18)
O22T—Mo5—O4C	154.94 (18)	Co1—O2C—Mo3	104.42 (17)
O11B—Mo5—O4C	85.68 (16)	Mo2—O2C—Mo3	90.92 (15)
O10B—Mo5—O4C	69.90 (15)	Co1—O3C—Mo3	104.78 (17)
O21T—Mo5—O5C	161.85 (17)	Co1—O3C—Mo4	103.09 (17)
O22T—Mo5—O5C	91.50 (17)	Mo3—O3C—Mo4	91.48 (15)
O11B—Mo5—O5C	73.56 (16)	Co1—O4C—Mo4	104.91 (18)
O10B—Mo5—O5C	81.08 (16)	Co1—O4C—Mo5	104.39 (18)
O4C—Mo5—O5C	68.21 (15)	Mo4—O4C—Mo5	97.09 (15)
O24T—Mo6—O23T	107.2 (2)	Co1—O5C—Mo5	103.25 (18)
O24T—Mo6—O12B	101.4 (2)	Co1—O5C—Mo6	103.77 (17)
O23T—Mo6—O12B	97.07 (19)	Mo5—O5C—Mo6	90.68 (15)
O24T—Mo6—O11B	97.3 (2)	Co1—O6C—Mo6	105.19 (18)
O23T—Mo6—O11B	100.39 (19)	Co1—O6C—Mo1	103.42 (18)
O12B—Mo6—O11B	149.29 (18)	Mo6—O6C—Mo1	90.73 (15)
O24T—Mo6—O6C	94.50 (19)	Mo1—O7B—O10B^{ix}	119.0 (2)
O23T—Mo6—O6C	157.64 (19)	Mo2—O7B—O10B^{ix}	122.7 (2)
O12B—Mo6—O6C	72.95 (16)	H1A—O1W—H1B	103 (4)
O11B—Mo6—O6C	81.53 (16)	H2A—O2W—H2B	106 (4)
O24T—Mo6—O5C	159.63 (19)	H3A—O3W—H3B	109 (4)
O23T—Mo6—O5C	92.00 (18)	H4A—O4W—H4B	108 (4)
O12B—Mo6—O5C	82.35 (16)	H5A—O5W—H5B	107 (5)
O11B—Mo6—O5C	72.04 (16)	H6A—O6W—H6B	107 (4)
O6C—Mo6—O5C	67.21 (14)	H7A—O7W—H7B	110 (5)
O2C—Co1—O1C	83.63 (18)	H8A—O8W—H8B	112 (4)
O2C—Co1—O6C	96.33 (18)		

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*−1/2; (ii) −*x*+1, −*y*, −*z*+1; (iii) *x*+1/2, −*y*+1/2, *z*−1/2; (iv) −*x*+1/2, *y*−1/2, −*z*+1/2; (v) *x*−1, *y*, *z*; (vi) −*x*, −*y*+1, −*z*+1; (vii) *x*−1/2, −*y*+1/2, *z*+1/2; (viii) −*x*+1/2, *y*−1/2, −*z*+3/2; (ix) *x*+1/2, −*y*+1/2, *z*+1/2; (x) *x*+1, *y*, *z*; (xi) −*x*+1/2, *y*+1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*C*—H1···O2*W*	0.85 (3)	1.81 (3)	2.639 (6)	167 (7)
O2*C*—H2···O22*T*^{ix}	0.81 (3)	1.98 (3)	2.787 (6)	170 (7)
O3*C*—H3···O6*W*	0.84 (3)	1.99 (4)	2.775 (6)	154 (6)
O4*C*—H4···O8*W*	0.84 (3)	1.81 (3)	2.627 (6)	165 (7)
O5*C*—H5···O15*T*^{i}	0.83 (3)	1.99 (3)	2.822 (6)	171 (7)
O6*C*—H6···O7*W*	0.82 (3)	1.96 (3)	2.761 (6)	165 (7)
O7*B*—H7···O10*B*^{ix}	1.21 (2)	1.22 (2)	2.430 (5)	175 (6)
O1*W*—H1*B*···O14*T*	0.86 (3)	1.89 (4)	2.731 (7)	163 (8)
O1*W*—H1*A*···O16*T*	0.85 (3)	2.18 (5)	2.878 (7)	140 (6)

O2*W*—H2*A*···O8*W*^{iii}	0.85 (3)	1.91 (3)	2.757 (6)	176 (7)
O2*W*—H2*B*···O15*T*^{i}	0.83 (3)	2.13 (4)	2.841 (6)	145 (6)
O3*W*—H3*B*···O19*T*	0.83 (3)	2.01 (3)	2.792 (7)	156 (6)
O3*W*—H3*A*···O1*W*^{i}	0.83 (3)	2.02 (4)	2.784 (7)	154 (8)
O4*W*—H4*A*···O23*T*^{ix}	0.84 (3)	1.97 (3)	2.800 (6)	167 (7)
O4*W*—H4*B*···O9*B*	0.84 (3)	1.91 (3)	2.734 (6)	167 (7)
O6*W*—H6*B*···O3*W*	0.84 (3)	1.88 (3)	2.709 (7)	169 (7)
O6*W*—H6*A*···O11*B*^{iii}	0.83 (3)	2.31 (6)	2.921 (6)	131 (6)
O7*W*—H7*A*···O8*B*^{vii}	0.81 (3)	2.42 (6)	2.937 (6)	122 (6)
O7*W*—H7*B*···O6*W*^{vii}	0.82 (3)	2.00 (3)	2.811 (7)	166 (8)
O8*W*—H8*B*···O4*W*	0.83 (3)	1.88 (3)	2.697 (7)	168 (7)
O8*W*—H8*A*···O7*W*	0.82 (3)	2.01 (4)	2.761 (8)	151 (7)

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