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Heptaguanidinium sodium bis(pentaaquatetracosaoxoheptamolybdocobaltate) octahydrate

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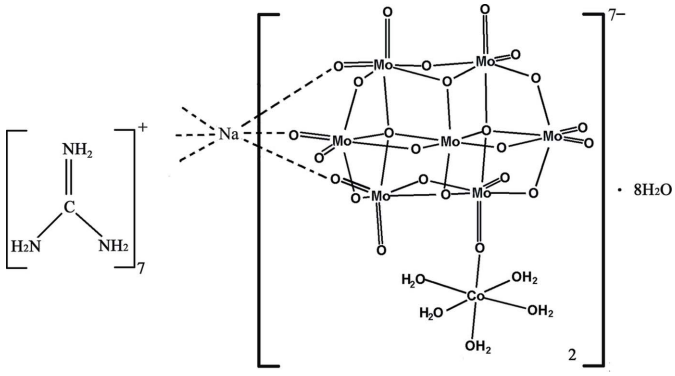
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(N–C) = 0.016 Å; disorder in solvent or counterion; R factor = 0.041; wR factor = 0.096; data-to-parameter ratio = 14.7.

The title compound, $(CH_6N_3)_7Na[CoMo_7O_{24}(H_2O)_5]_2\cdot 8H_2O$, features unusual $[Co(H_2O)_5Mo_7O_{24}]^{4-}$ polymetallate anions. Two such anions are connected by a bridging octahedral sodium ion (Na site symmetry $\overline{1}$) to form an $\{Na[(Co(H_2O)_5)(Mo_7O_{24})]_2\}^{7-}$ cluster. The Co—O and Mo—O distances are in the ranges 2.081 (11)–2.121 (10) and 1.701 (8)–2.508 (7) Å, respectively. Together with the cluster, the charge-balancing guanidinium cations (one of which is disordered about an inversion centre) and isolated water molecules form a three-dimensional supramolecular network by way of numerous O—H···O and N—H···O hydrogen bonds.

Related literature

For related structures, see: Liu, Li *et al.* (2006); Liu, Zhou *et al.*, (2006). For related literature, see: Brown & Altermatt (1985).



Experimental

Crystal data

$(CH_6N_3)_7Na[CoMo_7O_{24}(H_2O)_5]_2\cdot 8H_2O$
M_r = 2996.92
Monoclinic, $P2_1/c$
a = 18.819 (3) Å
b = 10.581 (2) Å
c = 19.926 (3) Å
β = 102.635 (2)°
V = 3871.7 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.73 mm^{-1}
T = 293 (2) K
0.28 × 0.22 × 0.16 mm

Data collection

Bruker SMART CCD APEX II diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.485, T_{max} = 0.650
19853 measured reflections
7505 independent reflections
4569 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.096
S = 0.99
7505 reflections
511 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 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
OW1—H1···OW5	0.89	2.33	2.988 (15)	131
OW1—H2···OW8	0.85	2.14	2.827 (15)	139
OW1—H1···O20^{i}	0.89	2.05	2.837 (12)	147
OW2—H3···OW7	0.83	1.97	2.795 (17)	170
OW2—H4···O21^{ii}	0.82	2.07	2.859 (12)	162
OW3—H5···O23^{iii}	0.83	2.29	2.778 (12)	118
OW3—H5···O23^{iii}	0.83	2.29	2.778 (12)	118
OW4—H8···OW1	1.01	2.15	2.879 (13)	128
OW4—H8···OW8^{i}	1.01	2.35	2.879 (16)	112
OW4—H7···O22^{iii}	0.79	2.48	2.793 (11)	106
OW5—H10···OW4	1.00	2.49	3.029 (16)	114
OW5—H9···O20^{ii}	0.89	2.04	2.849 (15)	150
OW6—H11···O6	0.81	2.35	2.993 (14)	136
OW6—H12···OW7^{i}	0.88	2.42	3.123 (17)	136
OW7—H13···O2	0.87	2.02	2.767 (13)	144
OW7—H14···OW9	0.92	2.10	2.98 (2)	161
OW8—H16···O6	0.83	2.50	2.791 (13)	102
OW8—H16···O6	0.83	2.50	2.791 (13)	102
OW8—H16···OW7	0.83	2.28	2.965 (19)	140
OW9—H17···OW6^{iv}	1.00	2.22	3.00 (2)	134
OW9—H18···OW2^{v}	1.00	2.30	3.111 (18)	137
N1—H1A···O8	0.86	2.22	2.968 (11)	145
N1—H1B···O10^{vi}	0.86	2.14	2.967 (11)	161
N2—H2A···O9^{iii}	0.86	2.18	2.992 (11)	157
N2—H2B···O8	0.86	2.18	2.936 (11)	147
N3—H3A···O9^{iii}	0.86	2.48	3.216 (11)	144
N3—H3A···O10^{iii}	0.86	2.28	3.031 (11)	145
N3—H3B···O13^{vi}	0.86	2.35	3.128 (11)	151
N4—H4B···O5^{vii}	0.86	2.31	2.954 (12)	131
N4—H4A···O12	0.86	2.09	2.918 (12)	160
N5—H5A···O4	0.86	2.11	2.965 (11)	177
N5—H5B···O17^{viii}	0.86	2.18	3.011 (12)	161
N6—H6A···O19^{viii}	0.86	2.37	2.864 (12)	117
N7—H7B···O7	0.86	2.42	3.175 (13)	147
N7—H7B···O14	0.86	2.37	3.107 (13)	144
N8—H8A···O16^{ix}	0.86	2.16	2.952 (13)	153
N8—H8B···OW6^{ii}	0.86	2.18	2.992 (18)	157
N9—H9A···O11^{ix}	0.86	2.09	2.918 (14)	162
N9—H9B···O7	0.86	2.18	2.992 (13)	157
N10—H10A···O12^{ix}	0.86	2.26	3.100 (13)	167
N10—H10B···O5	0.86	2.29	2.960 (12)	135
N11—H11B···O24^{viii}	0.86	2.22	2.935 (15)	141
N11—H11A···O19^{ix}	0.86	2.09	2.916 (16)	160

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $x, y+1, z$; (iv) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$; (v) $-x, -y+1, -z+1$; (vi) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (vii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (viii) $x, y-1, z$; (ix) $x, -y+\frac{1}{2}, z+\frac{1}{2}$.

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Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *DIAMOND* (Brandenburg, 1999); 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: HB2415).

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supplementary materials

Acta Cryst. (2007). E**63**, m1911-m1912 [**doi:10.1107/S1600536807028772**]

Heptaguanidinium sodium bis(pentaaquatetracosaoxoheptamolybdocobaltate) octahydrate

C.-B. Li

Comment

In the syntheses of new polyoxometalates (POMs), varying the organic ligand used in the reaction was demonstrated to be an effective strategy (Liu, Li *et al.*, 2006; (Liu, Zhou *et al.*, 2006). As an extension of this work, we have combined sodium molybdate, cobalt(II) acetate, and guanidinium nitrate to yield the title compound, (I), (Fig. 1).

Compound (I) contains a $[Co(H_2O)_5Mo_7O_{24}]^{4-}$ anion, which is constructed from seven MoO_6 and one CoO_6 octahedra. The Co atom is coordinated by five water molecule O atoms and the remaining position is provided with a terminal oxygen atom from a MoO_6 octahedron. The Co—O and Mo—O distances range from 2.075 (10)–2.121 (9) and 1.696 (7)–2.506 (7) Å, respectively. Bond-valence sum calculations (Brown & Altermatt, 1985) indicate oxidation states of 5.78–6.16 for Mo and 2.01 for Co, in agreement with the expected values of 6 and 2. Adjacent $[Co(H_2O)_5Mo_7O_{24}]^{4-}$ anions share a Na^+ ion (site symmetry $\bar{1}$) to form a dimeric $[Na(Co(H_2O)_5Mo_7O_{24})_2]^{7-}$ anionic cluster. The sodium cation displays a distorted NaO_6 octahedron coordinated by six terminal oxygen atoms from two neighboring $[Co(H_2O)_5Mo_7O_{24}]^{4-}$ anions.

The anions, charge balancing guanidinium cations (one of which is is disordered about an inversion centre) and isolated water molecules interact by way of a large number of N—H···O and O—H···O hydrogen-bonding interactions (Table 2), thus forming a three-dimensional supramolecular network as shown in Fig. 2.

Experimental

$NaMoO_4{\cdot}2H_2O$ (1.0 g, 4.1 mmol) and $Co(CH_3COO)_2{\cdot}4H_2O$ (0.1 g, 0.4 mmol) were dissolved in 20 ml water with stirring. $CN_3H_{6.N}O_3$ (0.25 g, 2 mmol) was then added to the solution and the pH was adjusted to about 5.0–5.1 by adding 4 *M* HCl. The mixture was refluxed at 333 K for about 3 h and cooled to room temperature; the solution was then filtrated into a 50-ml beaker. Slow evaporation of the solvent at room temperature led to pink block-shaped crystals of (I) suitable for X-ray diffraction after one weeks.

Refinement

The C4-containing guanidinium cation is disordered about an inversion centre and its gemoetrical parameters are less certain than those of the other species.

The N-bound H atoms were positioned geometrically (N—H = 0.86 Å) and refined as riding with $U_{iso} = 1.2U_{eq}$(N).

The O-bound H atoms were located in difference maps and refined as riding in their as-found relative positions with $U_{iso} = 1.2U_{eq}$ (O—H = 0.79—1.01 Å). In a structure of this complexity, these H atom locations should be rearded as tentative.

Figures

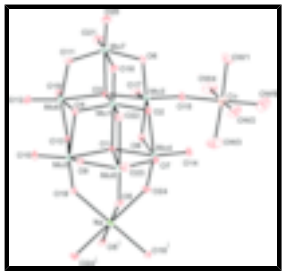

Fig. 1. A view of the anionic cluster in (I). Displacement ellipsoids are drawn at the 30% probability level (H atoms, guanidinium cations and uncoordinated water molecules omitted for clarity) [Symmetry code: (i) $1-x$, $1-y$, $1-z$].

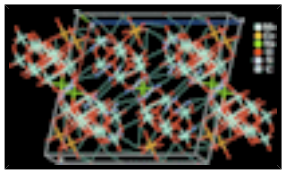

Fig. 2. The packing diagram of (I) (hydrogen bonds indicated by dashed lines).

Heptaguanidinium sodium bis(pentaaquatetracosaoxoheptamolybdocobaltate) octahydrate

Crystal data

$(CH_6N_3)_7Na[CoMo_7O_{24}(H_2O)_5]_2\cdot 8H_2O$	$F_{000} = 2896$
$M_r = 2996.92$	$D_x = 2.571$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 4954 reflections
$a = 18.819$ (3) Å	$\theta = 2.0$–27.5º
$b = 10.581$ (2) Å	$\mu = 2.73$ mm^{-1}
$c = 19.926$ (3) Å	$T = 293$ (2) K
$\beta = 102.635$ (2)º	Block, pink
$V = 3871.7$ (11) Å^3	0.28 × 0.22 × 0.16 mm
$Z = 2$	

Data collection

Bruker SMART CCD APEX II diffractometer	7505 independent reflections
Radiation source: fine-focus sealed tube	4569 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.074$
Detector resolution: not measured pixels mm^{-1}	$\theta_{max} = 26.0$º
$T = 293(2)$ K	$\theta_{min} = 2.2$º
ω and φ scans	$h = -23\rightarrow16$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$k = -13\rightarrow13$
$T_{min} = 0.485$, $T_{max} = 0.650$	$l = -19\rightarrow24$
19853 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.096$	$w = 1/[\sigma^2(F_o^2) + (0.0671P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{max} < 0.001$
7505 reflections	$\Delta\rho_{max} = 0.68$ e Å^{-3}
511 parameters	$\Delta\rho_{min} = -0.55$ 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}	Occ. (<1)
Mo1	0.23286 (5)	0.40375 (8)	0.29023 (5)	0.0206 (2)	
Mo2	0.41916 (5)	0.38005 (8)	0.32096 (5)	0.0204 (2)	
Mo3	0.21258 (5)	0.72412 (8)	0.29143 (5)	0.0230 (2)	
Mo4	0.29702 (5)	0.58470 (8)	0.43326 (5)	0.0223 (2)	
Mo5	0.33991 (5)	0.29401 (8)	0.43889 (5)	0.0226 (2)	
Mo6	0.33209 (5)	0.51210 (8)	0.17789 (5)	0.0219 (2)	
Mo7	0.16280 (5)	0.58368 (9)	0.14662 (5)	0.0274 (2)	
Co	0.11521 (10)	0.92346 (17)	0.39784 (10)	0.0468 (5)	
Na	0.5000	0.5000	0.5000	0.0334 (15)	
O1	0.3355 (3)	0.4504 (6)	0.3687 (3)	0.0174 (14)	
O2	0.2043 (3)	0.5356 (6)	0.3437 (4)	0.0244 (16)	
O3	0.2534 (3)	0.5821 (6)	0.2332 (3)	0.0195 (15)	
O4	0.3070 (3)	0.3544 (6)	0.2460 (3)	0.0210 (15)	
O5	0.4182 (4)	0.3265 (7)	0.5009 (4)	0.0291 (17)	
O6	0.1292 (3)	0.6644 (7)	0.2197 (4)	0.0276 (17)	
O7	0.2766 (4)	0.4170 (6)	0.4667 (4)	0.0266 (17)	
O8	0.2994 (3)	0.7066 (6)	0.3606 (4)	0.0230 (16)	
O9	0.3850 (3)	0.2345 (6)	0.3678 (3)	0.0223 (15)	

O10	0.4597 (4)	0.2828 (6)	0.2713 (4)	0.0279 (17)
O11	0.2337 (4)	0.4758 (7)	0.1215 (4)	0.0323 (18)
O12	0.3756 (4)	0.4051 (7)	0.1354 (4)	0.0318 (18)
O13	0.4039 (3)	0.5263 (6)	0.2629 (3)	0.0221 (15)
O14	0.2396 (4)	0.6598 (7)	0.4755 (4)	0.0333 (18)
O15	0.1561 (4)	0.7910 (7)	0.3388 (4)	0.0358 (19)
O16	0.1561 (4)	0.3929 (7)	0.2242 (4)	0.0325 (18)
O17	0.2389 (4)	0.8481 (7)	0.2483 (4)	0.038 (2)
O18	0.4892 (4)	0.4353 (7)	0.3844 (4)	0.0286 (17)
O19	0.3473 (4)	0.6553 (6)	0.1447 (4)	0.0328 (18)
O20	0.0851 (4)	0.5101 (8)	0.1010 (4)	0.045 (2)
O21	0.1733 (4)	0.7153 (7)	0.0994 (4)	0.040 (2)
O22	0.2293 (4)	0.2733 (6)	0.3430 (4)	0.0306 (17)
O23	0.3049 (4)	0.1576 (7)	0.4644 (4)	0.0365 (19)
O24	0.3843 (4)	0.6113 (7)	0.4815 (4)	0.0337 (18)
OW1	0.0144 (4)	0.8959 (9)	0.3291 (5)	0.059 (3)
H1	0.0002	0.9427	0.3611	0.071*
H2	0.0022	0.8188	0.3280	0.071*
OW2	0.0921 (5)	0.7733 (9)	0.4603 (5)	0.043 (3)
H3	0.0926	0.7055	0.4391	0.052*
H4	0.1233	0.7761	0.4962	0.052*
OW3	0.2183 (5)	0.9444 (9)	0.4619 (6)	0.048 (3)
H5	0.2468	0.9682	0.4381	0.058*
H6	0.2252	0.9938	0.4934	0.058*
OW4	0.1321 (5)	1.0711 (8)	0.3324 (5)	0.044 (3)
H7	0.1225	1.1381	0.3452	0.053*
H8	0.0918	1.0234	0.3012	0.053*
OW5	0.0675 (6)	1.0433 (11)	0.4582 (6)	0.057 (3)
H10	0.0770	1.1195	0.4321	0.068*
H9	0.0893	1.0200	0.5008	0.068*
OW6	0.0746 (7)	0.9225 (12)	0.1733 (9)	0.138 (6)
H11	0.1078	0.8720	0.1779	0.166*
H12	0.0286	0.9327	0.1757	0.166*
OW7	0.0768 (6)	0.5417 (13)	0.3912 (7)	0.104 (4)
H13	0.1182	0.5098	0.3877	0.124*
H14	0.0616	0.4852	0.4204	0.124*
OW8	−0.0030 (6)	0.6593 (11)	0.2614 (7)	0.094 (4)
H15	−0.0015	0.6459	0.2154	0.113*
H16	0.0315	0.6172	0.2830	0.113*
OW9	0.0197 (8)	0.3218 (14)	0.4569 (8)	0.132 (5)
H17	−0.0119	0.3036	0.4109	0.158*
H18	−0.0256	0.3354	0.4743	0.158*
N1	0.4305 (5)	0.7968 (8)	0.3149 (5)	0.038 (2)
H1A	0.4026	0.7406	0.3268	0.046*
H1B	0.4638	0.7745	0.2938	0.046*
N2	0.3716 (4)	0.9528 (8)	0.3612 (5)	0.031 (2)
H2A	0.3648	1.0315	0.3685	0.037*
H2B	0.3450	0.8964	0.3749	0.037*
N3	0.4635 (5)	1.0043 (8)	0.3075 (5)	0.034 (2)

H3A	0.4572	1.0833	0.3146	0.041*	
H3B	0.4967	0.9809	0.2865	0.041*	
N4	0.3851 (5)	0.1298 (9)	0.1373 (5)	0.042 (3)	
H4A	0.3842	0.2087	0.1475	0.051*	
H4B	0.4112	0.1044	0.1095	0.051*	
N5	0.3072 (5)	0.0844 (9)	0.2063 (5)	0.040 (3)	
H5A	0.3054	0.1627	0.2172	0.048*	
H5B	0.2825	0.0292	0.2233	0.048*	
N6	0.3486 (6)	−0.0740 (9)	0.1460 (6)	0.056 (3)	
H6A	0.3232	−0.1286	0.1625	0.067*	
H6B	0.3750	−0.0977	0.1180	0.067*	
N7	0.1706 (6)	0.4791 (11)	0.5664 (6)	0.060 (3)	
H7A	0.1474	0.5386	0.5818	0.072*	
H7B	0.1951	0.4954	0.5357	0.072*	
N8	0.1343 (6)	0.3325 (12)	0.6347 (6)	0.062 (3)	
H8A	0.1342	0.2550	0.6476	0.075*	
H8B	0.1108	0.3885	0.6524	0.075*	
N9	0.2033 (6)	0.2764 (11)	0.5629 (6)	0.059 (3)	
H9A	0.2022	0.1996	0.5768	0.071*	
H9B	0.2273	0.2951	0.5322	0.071*	
N10	0.4687 (5)	0.0622 (10)	0.5260 (5)	0.051 (3)	
H10A	0.4377	0.0766	0.5511	0.062*	
H10B	0.4801	0.1389	0.5186	0.062*	
N11	0.4383 (7)	−0.1460 (12)	0.5436 (7)	0.012 (3)	0.50
H11A	0.4099	−0.1289	0.5710	0.014*	0.50
H11B	0.4449	−0.2232	0.5329	0.014*	0.50
C1	0.4223 (6)	0.9190 (10)	0.3290 (5)	0.029 (3)	
C2	0.3473 (6)	0.0494 (10)	0.1641 (6)	0.031 (3)	
C3	0.1687 (7)	0.3640 (14)	0.5888 (7)	0.048 (3)	
C4	0.4765 (12)	−0.057 (2)	0.5158 (12)	0.029 (5)	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.0210 (5)	0.0199 (5)	0.0215 (5)	−0.0035 (4)	0.0058 (4)	−0.0004 (4)
Mo2	0.0212 (5)	0.0191 (5)	0.0213 (5)	0.0009 (4)	0.0056 (4)	−0.0018 (4)
Mo3	0.0230 (5)	0.0217 (5)	0.0254 (5)	0.0036 (4)	0.0073 (4)	0.0016 (4)
Mo4	0.0248 (5)	0.0217 (5)	0.0208 (5)	0.0043 (4)	0.0060 (4)	−0.0017 (4)
Mo5	0.0265 (5)	0.0187 (5)	0.0227 (5)	0.0000 (4)	0.0059 (4)	0.0033 (4)
Mo6	0.0239 (5)	0.0214 (5)	0.0216 (5)	0.0000 (4)	0.0075 (4)	0.0003 (4)
Mo7	0.0224 (5)	0.0368 (6)	0.0216 (5)	−0.0013 (4)	0.0019 (4)	0.0034 (4)
Co	0.0481 (11)	0.0433 (11)	0.0491 (12)	0.0022 (8)	0.0112 (8)	−0.0018 (9)
Na	0.028 (3)	0.035 (4)	0.038 (4)	0.000 (3)	0.008 (3)	−0.010 (3)
O1	0.018 (3)	0.017 (3)	0.017 (4)	0.000 (3)	0.003 (3)	0.004 (3)
O2	0.022 (4)	0.022 (4)	0.031 (4)	−0.005 (3)	0.010 (3)	−0.003 (3)
O3	0.023 (4)	0.019 (3)	0.016 (4)	0.002 (3)	0.004 (3)	0.004 (3)
O4	0.025 (4)	0.018 (4)	0.019 (4)	−0.001 (3)	0.003 (3)	0.001 (3)
O5	0.033 (4)	0.032 (4)	0.020 (4)	−0.001 (3)	0.000 (3)	0.001 (3)

O6	0.021 (4)	0.029 (4)	0.033 (5)	0.003 (3)	0.007 (3)	0.001 (3)
O7	0.026 (4)	0.034 (4)	0.023 (4)	0.007 (3)	0.012 (3)	0.006 (3)
O8	0.020 (4)	0.019 (4)	0.030 (4)	0.001 (3)	0.008 (3)	0.000 (3)
O9	0.028 (3)	0.013 (3)	0.026 (3)	−0.001 (3)	0.006 (3)	0.000 (3)
O10	0.035 (4)	0.022 (4)	0.032 (4)	0.004 (3)	0.018 (3)	−0.002 (3)
O11	0.020 (4)	0.045 (5)	0.030 (5)	0.006 (3)	0.000 (3)	−0.003 (4)
O12	0.038 (4)	0.038 (4)	0.021 (4)	0.004 (3)	0.008 (3)	0.002 (3)
O13	0.021 (4)	0.024 (4)	0.022 (4)	−0.003 (3)	0.010 (3)	0.000 (3)
O14	0.037 (4)	0.033 (4)	0.035 (5)	0.015 (4)	0.018 (4)	0.007 (4)
O15	0.035 (5)	0.039 (5)	0.035 (5)	0.016 (4)	0.011 (4)	−0.003 (4)
O16	0.032 (4)	0.037 (4)	0.028 (5)	−0.003 (3)	0.005 (3)	−0.005 (4)
O17	0.045 (5)	0.027 (4)	0.042 (5)	−0.003 (4)	0.010 (4)	0.001 (4)
O18	0.025 (4)	0.041 (4)	0.020 (4)	0.003 (3)	0.004 (3)	−0.002 (3)
O19	0.038 (5)	0.019 (4)	0.043 (5)	0.003 (3)	0.012 (4)	0.005 (3)
O20	0.032 (5)	0.069 (6)	0.031 (5)	−0.004 (4)	0.002 (4)	−0.002 (4)
O21	0.046 (5)	0.038 (5)	0.037 (5)	0.001 (4)	0.009 (4)	0.010 (4)
O22	0.038 (4)	0.027 (4)	0.027 (4)	−0.004 (3)	0.008 (3)	0.002 (3)
O23	0.040 (5)	0.028 (4)	0.040 (5)	−0.010 (4)	0.004 (4)	0.005 (4)
O24	0.030 (4)	0.034 (4)	0.032 (5)	0.007 (3)	−0.004 (3)	0.001 (4)
OW1	0.035 (5)	0.062 (6)	0.080 (8)	0.012 (4)	0.010 (5)	−0.001 (6)
OW2	0.066 (7)	0.039 (6)	0.020 (6)	0.000 (5)	0.001 (5)	0.003 (5)
OW3	0.048 (7)	0.039 (6)	0.049 (7)	−0.017 (5)	−0.009 (5)	0.009 (5)
OW4	0.055 (7)	0.023 (5)	0.048 (7)	−0.016 (5)	−0.005 (5)	0.005 (5)
OW5	0.065 (5)	0.056 (5)	0.050 (5)	0.002 (4)	0.011 (4)	0.005 (4)
OW6	0.082 (10)	0.115 (11)	0.209 (18)	0.021 (8)	0.011 (10)	0.068 (12)
OW7	0.067 (8)	0.142 (11)	0.113 (11)	−0.014 (8)	0.044 (7)	−0.013 (9)
OW8	0.089 (5)	0.098 (5)	0.095 (6)	−0.004 (4)	0.021 (4)	−0.011 (4)
OW9	0.128 (7)	0.134 (7)	0.132 (7)	−0.005 (5)	0.024 (5)	0.002 (5)
N1	0.044 (6)	0.023 (5)	0.056 (7)	0.002 (4)	0.028 (5)	−0.002 (5)
N2	0.024 (5)	0.029 (5)	0.044 (6)	0.000 (4)	0.017 (4)	−0.006 (4)
N3	0.032 (5)	0.017 (5)	0.056 (7)	−0.002 (4)	0.016 (5)	0.001 (5)
N4	0.065 (7)	0.026 (5)	0.043 (7)	−0.004 (5)	0.026 (5)	−0.008 (5)
N5	0.049 (6)	0.026 (5)	0.047 (7)	0.004 (5)	0.013 (5)	0.010 (5)
N6	0.080 (9)	0.037 (6)	0.057 (8)	0.004 (6)	0.030 (6)	−0.014 (6)
N7	0.053 (7)	0.065 (8)	0.070 (9)	0.014 (6)	0.030 (6)	0.043 (7)
N8	0.073 (8)	0.067 (8)	0.058 (8)	0.002 (7)	0.040 (7)	0.027 (7)
N9	0.056 (8)	0.059 (8)	0.067 (9)	−0.003 (6)	0.024 (6)	0.007 (7)
N10	0.048 (7)	0.067 (8)	0.037 (7)	0.020 (6)	0.004 (5)	0.002 (6)
N11	0.012 (3)	0.012 (3)	0.012 (3)	−0.0001 (10)	0.0028 (12)	−0.0008 (10)
C1	0.032 (6)	0.035 (6)	0.016 (6)	0.004 (5)	−0.002 (5)	−0.005 (5)
C2	0.053 (8)	0.019 (6)	0.022 (6)	0.010 (5)	0.011 (5)	−0.003 (5)
C3	0.037 (8)	0.060 (9)	0.048 (9)	0.016 (7)	0.010 (6)	0.022 (7)
C4	0.030 (6)	0.026 (6)	0.030 (7)	0.004 (5)	0.002 (5)	−0.004 (5)

Geometric parameters (Å, °)

Mo1—O16	1.732 (7)	OW1—H2	0.8455
Mo1—O22	1.745 (7)	OW2—H3	0.8334
Mo1—O4	1.880 (7)	OW2—H4	0.8210

Mo1—O2	1.903 (7)	OW3—H5	0.8290
Mo1—O1	2.258 (6)	OW3—H6	0.8066
Mo1—O3	2.279 (6)	OW4—H7	0.7875
Mo2—O10	1.717 (7)	OW4—H8	1.0051
Mo2—O18	1.717 (7)	OW5—H10	0.9960
Mo2—O13	1.916 (7)	OW5—H9	0.8934
Mo2—O9	1.980 (6)	OW6—H11	0.8123
Mo2—O1	2.142 (6)	OW6—H12	0.8843
Mo2—O4	2.320 (6)	OW7—H13	0.8657
Mo3—O17	1.701 (8)	OW7—H14	0.9208
Mo3—O15	1.720 (7)	OW8—H15	0.9342
Mo3—O8	1.901 (7)	OW8—H16	0.8261
Mo3—O6	1.980 (7)	OW9—H17	0.9962
Mo3—O3	2.141 (6)	OW9—H18	0.9975
Mo3—O2	2.271 (7)	N1—C1	1.340 (13)
Mo4—O14	1.704 (7)	N1—H1A	0.8600
Mo4—O24	1.735 (7)	N1—H1B	0.8600
Mo4—O8	1.947 (7)	N2—C1	1.310 (13)
Mo4—O7	1.963 (7)	N2—H2A	0.8600
Mo4—O1	2.147 (6)	N2—H2B	0.8600
Mo4—O2	2.266 (7)	N3—C1	1.321 (13)
Mo5—O23	1.709 (7)	N3—H3A	0.8600
Mo5—O5	1.737 (7)	N3—H3B	0.8600
Mo5—O9	1.910 (7)	N4—C2	1.297 (14)
Mo5—O7	1.926 (7)	N4—H4A	0.8600
Mo5—O1	2.156 (6)	N4—H4B	0.8600
Mo5—O22	2.508 (7)	N5—C2	1.301 (14)
Mo6—O19	1.702 (7)	N5—H5A	0.8600
Mo6—O12	1.724 (7)	N5—H5B	0.8600
Mo6—O13	1.928 (7)	N6—C2	1.357 (13)
Mo6—O11	1.983 (7)	N6—H6A	0.8600
Mo6—O3	2.161 (6)	N6—H6B	0.8600
Mo6—O4	2.265 (6)	N7—C3	1.301 (16)
Mo7—O21	1.716 (8)	N7—H7A	0.8600
Mo7—O20	1.729 (8)	N7—H7B	0.8600
Mo7—O11	1.905 (7)	N8—C3	1.275 (16)
Mo7—O6	1.912 (7)	N8—H8A	0.8600
Mo7—O3	2.144 (6)	N8—H8B	0.8600
Co—OW5	2.081 (11)	N9—C3	1.302 (16)
Co—O15	2.082 (7)	N9—H9A	0.8600
Co—OW3	2.087 (9)	N9—H9B	0.8600
Co—OW4	2.103 (9)	N10—C4	1.29 (2)
Co—OW1	2.103 (9)	N10—C4^{ii}	1.46 (2)
Co—OW2	2.121 (10)	N10—H10A	0.8600
Na—O18	2.369 (7)	N10—H10B	0.8605
Na—O18^{i}	2.369 (7)	N11—C4	1.37 (2)
Na—O5	2.399 (7)	N11—H11A	0.8600
Na—O5^{i}	2.399 (7)	N11—H11B	0.8600

Na—O24^{i}	2.431 (7)	C4—N10^{ii}	1.46 (2)
Na—O24	2.431 (7)	C4—C4^{ii}	1.70 (4)
OW1—H1	0.8926		
O16—Mo1—O22	105.7 (3)	O3—Mo7—Mo3	41.69 (17)
O16—Mo1—O4	101.9 (3)	O21—Mo7—Mo6	94.0 (3)
O22—Mo1—O4	101.1 (3)	O20—Mo7—Mo6	133.4 (3)
O16—Mo1—O2	100.6 (3)	O11—Mo7—Mo6	35.4 (2)
O22—Mo1—O2	100.9 (3)	O6—Mo7—Mo6	116.0 (2)
O4—Mo1—O2	142.7 (3)	O3—Mo7—Mo6	42.17 (17)
O16—Mo1—O1	170.3 (3)	Mo3—Mo7—Mo6	81.47 (3)
O22—Mo1—O1	84.0 (3)	OW5—Co—O15	174.8 (4)
O4—Mo1—O1	77.0 (3)	OW5—Co—OW3	92.4 (5)
O2—Mo1—O1	75.8 (3)	O15—Co—OW3	90.4 (4)
O16—Mo1—O3	83.1 (3)	OW5—Co—OW4	92.8 (4)
O22—Mo1—O3	171.2 (3)	O15—Co—OW4	91.4 (4)
O4—Mo1—O3	76.8 (2)	OW3—Co—OW4	93.1 (4)
O2—Mo1—O3	76.8 (3)	OW5—Co—OW1	91.1 (4)
O1—Mo1—O3	87.2 (2)	O15—Co—OW1	86.1 (3)
O10—Mo2—O18	105.2 (3)	OW3—Co—OW1	176.4 (4)
O10—Mo2—O13	99.4 (3)	OW4—Co—OW1	86.4 (4)
O18—Mo2—O13	99.2 (3)	OW5—Co—OW2	87.0 (4)
O10—Mo2—O9	92.1 (3)	O15—Co—OW2	88.6 (4)
O18—Mo2—O9	101.2 (3)	OW3—Co—OW2	90.2 (4)
O13—Mo2—O9	153.1 (3)	OW4—Co—OW2	176.8 (4)
O10—Mo2—O1	157.8 (3)	OW1—Co—OW2	90.4 (4)
O18—Mo2—O1	94.3 (3)	O18—Na—O18^{i}	180.000 (1)
O13—Mo2—O1	87.7 (3)	O18—Na—O5	82.4 (2)
O9—Mo2—O1	73.4 (2)	O18^{i}—Na—O5	97.6 (2)
O10—Mo2—O4	90.9 (3)	O18—Na—O5^{i}	97.6 (2)
O18—Mo2—O4	163.3 (3)	O18^{i}—Na—O5^{i}	82.4 (2)
O13—Mo2—O4	73.2 (2)	O5—Na—O5^{i}	180.0 (2)
O9—Mo2—O4	82.5 (2)	O18—Na—O24^{i}	83.8 (2)
O1—Mo2—O4	70.9 (2)	O18^{i}—Na—O24^{i}	96.2 (2)
O10—Mo2—Mo5	126.4 (2)	O5—Na—O24^{i}	100.6 (2)
O18—Mo2—Mo5	87.8 (2)	O5^{i}—Na—O24^{i}	79.4 (2)
O13—Mo2—Mo5	130.14 (19)	O18—Na—O24	96.2 (2)
O9—Mo2—Mo5	34.45 (19)	O18^{i}—Na—O24	83.8 (2)
O1—Mo2—Mo5	42.47 (16)	O5—Na—O24	79.4 (2)
O4—Mo2—Mo5	86.25 (16)	O5^{i}—Na—O24	100.6 (2)
O17—Mo3—O15	104.1 (4)	O24^{i}—Na—O24	180.000 (1)
O17—Mo3—O8	98.2 (3)	O18—Na—Mo5	67.64 (17)
O15—Mo3—O8	100.2 (3)	O18^{i}—Na—Mo5	112.36 (17)
O17—Mo3—O6	98.9 (3)	O5—Na—Mo5	22.23 (16)
O15—Mo3—O6	92.3 (3)	O5^{i}—Na—Mo5	157.77 (16)
O8—Mo3—O6	155.7 (3)	O24^{i}—Na—Mo5	113.72 (17)

O17—Mo3—O3	95.1 (3)	O24—Na—Mo5	66.28 (17)
O15—Mo3—O3	157.5 (3)	O18—Na—Mo5^{i}	112.36 (17)
O8—Mo3—O3	88.3 (3)	O18^{i}—Na—Mo5^{i}	67.64 (17)
O6—Mo3—O3	72.9 (3)	O5—Na—Mo5^{i}	157.77 (16)
O17—Mo3—O2	165.0 (3)	O5^{i}—Na—Mo5^{i}	22.23 (16)
O15—Mo3—O2	89.8 (3)	O24^{i}—Na—Mo5^{i}	66.28 (17)
O8—Mo3—O2	73.5 (3)	O24—Na—Mo5^{i}	113.72 (17)
O6—Mo3—O2	85.9 (3)	Mo5—Na—Mo5^{i}	180.00 (4)
O3—Mo3—O2	72.6 (2)	Mo2—O1—Mo4	150.8 (3)
O17—Mo3—Mo7	87.9 (3)	Mo2—O1—Mo5	95.4 (2)
O15—Mo3—Mo7	126.3 (3)	Mo4—O1—Mo5	95.1 (2)
O8—Mo3—Mo7	130.1 (2)	Mo2—O1—Mo1	102.5 (3)
O6—Mo3—Mo7	34.0 (2)	Mo4—O1—Mo1	102.1 (2)
O3—Mo3—Mo7	41.76 (17)	Mo5—O1—Mo1	100.8 (2)
O2—Mo3—Mo7	88.28 (18)	Mo1—O2—Mo4	110.3 (3)
O14—Mo4—O24	106.1 (4)	Mo1—O2—Mo3	109.3 (3)
O14—Mo4—O8	100.3 (3)	Mo4—O2—Mo3	92.4 (2)
O24—Mo4—O8	97.6 (3)	Mo3—O3—Mo7	96.5 (2)
O14—Mo4—O7	93.5 (3)	Mo3—O3—Mo6	152.2 (3)
O24—Mo4—O7	101.0 (3)	Mo7—O3—Mo6	96.0 (3)
O8—Mo4—O7	152.8 (3)	Mo3—O3—Mo1	101.0 (3)
O14—Mo4—O1	159.8 (3)	Mo7—O3—Mo1	102.4 (3)
O24—Mo4—O1	92.1 (3)	Mo6—O3—Mo1	100.4 (2)
O8—Mo4—O1	85.8 (3)	Mo1—O4—Mo6	110.5 (3)
O7—Mo4—O1	73.9 (3)	Mo1—O4—Mo2	109.2 (3)
O14—Mo4—O2	92.0 (3)	Mo6—O4—Mo2	91.1 (2)
O24—Mo4—O2	161.0 (3)	Mo5—O5—Na	126.3 (4)
O8—Mo4—O2	72.8 (3)	Mo7—O6—Mo3	110.5 (3)
O7—Mo4—O2	83.5 (3)	Mo5—O7—Mo4	109.5 (3)
O1—Mo4—O2	71.3 (2)	Mo3—O8—Mo4	116.6 (3)
O14—Mo4—Mo5	128.2 (3)	Mo5—O9—Mo2	109.6 (3)
O24—Mo4—Mo5	86.3 (2)	Mo7—O11—Mo6	110.8 (4)
O8—Mo4—Mo5	128.40 (19)	Mo2—O13—Mo6	116.8 (3)
O7—Mo4—Mo5	34.88 (19)	Mo3—O15—Co	159.4 (5)
O1—Mo4—Mo5	42.56 (16)	Mo2—O18—Na	134.7 (4)
O2—Mo4—Mo5	87.23 (17)	Mo1—O22—Mo5	104.8 (3)
O23—Mo5—O5	106.1 (3)	Mo4—O24—Na	135.5 (4)
O23—Mo5—O9	101.8 (3)	Co—OW1—H1	79.9
O5—Mo5—O9	98.5 (3)	Co—OW1—H2	110.6
O23—Mo5—O7	100.5 (3)	H1—OW1—H2	115.6
O5—Mo5—O7	98.2 (3)	Co—OW2—H3	108.7
O9—Mo5—O7	147.1 (3)	Co—OW2—H4	106.6
O23—Mo5—O1	151.4 (3)	H3—OW2—H4	112.9
O5—Mo5—O1	102.5 (3)	Co—OW3—H5	108.4
O9—Mo5—O1	74.5 (2)	Co—OW3—H6	121.1
O7—Mo5—O1	74.4 (3)	H5—OW3—H6	103.4
O23—Mo5—O22	81.0 (3)	Co—OW4—H7	113.1

O5—Mo5—O22	172.9 (3)	Co—OW4—H8	79.3
O9—Mo5—O22	80.5 (3)	H7—OW4—H8	117.1
O7—Mo5—O22	79.4 (3)	Co—OW5—H10	92.5
O1—Mo5—O22	70.4 (2)	Co—OW5—H9	102.4
O23—Mo5—Mo4	135.8 (3)	H10—OW5—H9	128.5
O5—Mo5—Mo4	90.2 (2)	H11—OW6—H12	144.4
O9—Mo5—Mo4	116.34 (19)	H13—OW7—H14	101.9
O7—Mo5—Mo4	35.7 (2)	H15—OW8—H16	103.9
O1—Mo5—Mo4	42.32 (17)	H17—OW9—H18	88.0
O22—Mo5—Mo4	84.00 (16)	C1—N1—H1A	120.2
O23—Mo5—Mo2	137.3 (3)	C1—N1—H1B	119.8
O5—Mo5—Mo2	90.4 (2)	H1A—N1—H1B	120.0
O9—Mo5—Mo2	35.90 (18)	C1—N2—H2A	119.8
O7—Mo5—Mo2	116.1 (2)	C1—N2—H2B	120.2
O1—Mo5—Mo2	42.14 (16)	H2A—N2—H2B	120.0
O22—Mo5—Mo2	84.67 (17)	C1—N3—H3A	119.9
Mo4—Mo5—Mo2	81.56 (3)	C1—N3—H3B	120.1
O23—Mo5—Na	137.6 (3)	H3A—N3—H3B	120.0
O5—Mo5—Na	31.5 (2)	C2—N4—H4A	119.9
O9—Mo5—Na	88.66 (19)	C2—N4—H4B	120.1
O7—Mo5—Na	91.0 (2)	H4A—N4—H4B	120.0
O1—Mo5—Na	71.01 (16)	C2—N5—H5A	119.9
O22—Mo5—Na	141.44 (16)	C2—N5—H5B	120.1
Mo4—Mo5—Na	67.89 (2)	H5A—N5—H5B	120.0
Mo2—Mo5—Na	66.11 (2)	C2—N6—H6A	120.0
O19—Mo6—O12	104.8 (4)	C2—N6—H6B	120.0
O19—Mo6—O13	97.3 (3)	H6A—N6—H6B	120.0
O12—Mo6—O13	99.6 (3)	C3—N7—H7A	120.5
O19—Mo6—O11	99.7 (3)	C3—N7—H7B	119.5
O12—Mo6—O11	94.5 (3)	H7A—N7—H7B	120.0
O13—Mo6—O11	154.4 (3)	C3—N8—H8A	119.9
O19—Mo6—O3	94.9 (3)	C3—N8—H8B	120.1
O12—Mo6—O3	158.0 (3)	H8A—N8—H8B	120.0
O13—Mo6—O3	87.2 (3)	C3—N9—H9A	119.8
O11—Mo6—O3	72.3 (3)	C3—N9—H9B	120.2
O19—Mo6—O4	164.4 (3)	H9A—N9—H9B	120.0
O12—Mo6—O4	89.7 (3)	C4—N10—C4^{ii}	75.9 (17)
O13—Mo6—O4	74.3 (2)	C4—N10—H10A	112.3
O11—Mo6—O4	84.6 (3)	C4^{ii}—N10—H10A	171.8
O3—Mo6—O4	72.0 (2)	C4—N10—H10B	148.4
O19—Mo6—Mo7	87.6 (2)	C4^{ii}—N10—H10B	72.6
O12—Mo6—Mo7	128.2 (2)	H10A—N10—H10B	99.3
O13—Mo6—Mo7	128.96 (19)	C4—N11—H11A	124.4
O11—Mo6—Mo7	33.8 (2)	C4—N11—H11B	115.6
O3—Mo6—Mo7	41.78 (17)	H11A—N11—H11B	120.0
O4—Mo6—Mo7	87.79 (16)	N2—C1—N3	121.0 (10)
O21—Mo7—O20	105.2 (4)	N2—C1—N1	119.7 (10)
O21—Mo7—O11	99.8 (4)	N3—C1—N1	119.2 (10)

O20—Mo7—O11	98.8 (4)	N4—C2—N5	121.8 (10)
O21—Mo7—O6	98.8 (3)	N4—C2—N6	118.6 (11)
O20—Mo7—O6	102.7 (3)	N5—C2—N6	119.5 (11)
O11—Mo7—O6	146.7 (3)	N8—C3—N7	123.2 (14)
O21—Mo7—O3	106.3 (3)	N8—C3—N9	118.3 (13)
O20—Mo7—O3	148.4 (3)	N7—C3—N9	118.5 (13)
O11—Mo7—O3	74.2 (3)	N10—C4—N11	121.1 (19)
O6—Mo7—O3	74.2 (3)	N10—C4—N10^{ii}	104.1 (16)
O21—Mo7—Mo3	94.1 (3)	N11—C4—N10^{ii}	134.8 (18)
O20—Mo7—Mo3	136.9 (3)	N10—C4—C4^{ii}	56.5 (13)
O11—Mo7—Mo3	115.6 (2)	N11—C4—C4^{ii}	177 (3)
O6—Mo7—Mo3	35.4 (2)	N10^{ii}—C4—C4^{ii}	47.6 (12)
O10—Mo2—O1—Mo4	−179.9 (7)	O4—Mo1—O3—Mo3	−157.6 (3)
O18—Mo2—O1—Mo4	28.6 (7)	O2—Mo1—O3—Mo3	−4.2 (3)
O13—Mo2—O1—Mo4	−70.4 (6)	O1—Mo1—O3—Mo3	−80.3 (3)
O9—Mo2—O1—Mo4	129.0 (7)	O16—Mo1—O3—Mo7	−0.9 (3)
O4—Mo2—O1—Mo4	−143.4 (7)	O4—Mo1—O3—Mo7	103.1 (3)
Mo5—Mo2—O1—Mo4	110.7 (7)	O2—Mo1—O3—Mo7	−103.5 (3)
O10—Mo2—O1—Mo5	69.5 (8)	O1—Mo1—O3—Mo7	−179.6 (3)
O18—Mo2—O1—Mo5	−82.0 (3)	O16—Mo1—O3—Mo6	−99.5 (3)
O13—Mo2—O1—Mo5	178.9 (3)	O4—Mo1—O3—Mo6	4.4 (3)
O9—Mo2—O1—Mo5	18.4 (2)	O2—Mo1—O3—Mo6	157.8 (3)
O4—Mo2—O1—Mo5	106.0 (3)	O1—Mo1—O3—Mo6	81.7 (3)
O10—Mo2—O1—Mo1	−32.8 (9)	O16—Mo1—O4—Mo6	75.5 (4)
O18—Mo2—O1—Mo1	175.7 (3)	O22—Mo1—O4—Mo6	−175.7 (3)
O13—Mo2—O1—Mo1	76.6 (3)	O2—Mo1—O4—Mo6	−50.4 (6)
O9—Mo2—O1—Mo1	−83.9 (3)	O1—Mo1—O4—Mo6	−94.6 (3)
O4—Mo2—O1—Mo1	3.7 (2)	O3—Mo1—O4—Mo6	−4.4 (3)
Mo5—Mo2—O1—Mo1	−102.3 (3)	O16—Mo1—O4—Mo2	174.3 (3)
O14—Mo4—O1—Mo2	177.5 (7)	O22—Mo1—O4—Mo2	−76.9 (3)
O24—Mo4—O1—Mo2	−28.5 (7)	O2—Mo1—O4—Mo2	48.4 (6)
O8—Mo4—O1—Mo2	68.9 (6)	O1—Mo1—O4—Mo2	4.2 (3)
O7—Mo4—O1—Mo2	−129.4 (7)	O3—Mo1—O4—Mo2	94.3 (3)
O2—Mo4—O1—Mo2	142.2 (7)	O19—Mo6—O4—Mo1	38.3 (12)
Mo5—Mo4—O1—Mo2	−110.7 (7)	O12—Mo6—O4—Mo1	−162.9 (4)
O14—Mo4—O1—Mo5	−71.8 (9)	O13—Mo6—O4—Mo1	97.0 (3)
O24—Mo4—O1—Mo5	82.2 (3)	O11—Mo6—O4—Mo1	−68.4 (3)
O8—Mo4—O1—Mo5	179.6 (3)	O3—Mo6—O4—Mo1	4.8 (3)
O7—Mo4—O1—Mo5	−18.6 (2)	O19—Mo6—O4—Mo2	−72.7 (11)
O2—Mo4—O1—Mo5	−107.1 (3)	O12—Mo6—O4—Mo2	86.0 (3)
O14—Mo4—O1—Mo1	30.4 (9)	O13—Mo6—O4—Mo2	−14.0 (2)
O24—Mo4—O1—Mo1	−175.6 (3)	O11—Mo6—O4—Mo2	−179.4 (3)
O8—Mo4—O1—Mo1	−78.2 (3)	O3—Mo6—O4—Mo2	−106.2 (3)
O7—Mo4—O1—Mo1	83.5 (3)	O10—Mo2—O4—Mo1	162.5 (3)
O2—Mo4—O1—Mo1	−4.9 (2)	O18—Mo2—O4—Mo1	−33.4 (11)
Mo5—Mo4—O1—Mo1	102.2 (3)	O13—Mo2—O4—Mo1	−98.0 (3)
O23—Mo5—O1—Mo2	−105.2 (7)	O9—Mo2—O4—Mo1	70.5 (3)
O5—Mo5—O1—Mo2	76.5 (3)	O1—Mo2—O4—Mo1	−4.5 (3)

O9—Mo5—O1—Mo2	−19.0 (2)	O10—Mo2—O4—Mo6	−85.4 (3)
O7—Mo5—O1—Mo2	171.7 (3)	O18—Mo2—O4—Mo6	78.8 (10)
O22—Mo5—O1—Mo2	−104.2 (3)	O13—Mo2—O4—Mo6	14.2 (2)
Mo4—Mo5—O1—Mo2	152.7 (3)	O9—Mo2—O4—Mo6	−177.3 (3)
Na—Mo5—O1—Mo2	75.05 (17)	O1—Mo2—O4—Mo6	107.6 (3)
O23—Mo5—O1—Mo4	102.1 (7)	O23—Mo5—O5—Na	178.2 (4)
O5—Mo5—O1—Mo4	−76.2 (3)	O9—Mo5—O5—Na	73.2 (4)
O9—Mo5—O1—Mo4	−171.7 (3)	O7—Mo5—O5—Na	−78.4 (4)
O7—Mo5—O1—Mo4	19.0 (3)	O1—Mo5—O5—Na	−2.7 (5)
O22—Mo5—O1—Mo4	103.0 (3)	O18—Na—O5—Mo5	−46.6 (4)
Mo2—Mo5—O1—Mo4	−152.7 (3)	O18^{i}—Na—O5—Mo5	133.4 (4)
Na—Mo5—O1—Mo4	−77.69 (17)	O24^{i}—Na—O5—Mo5	−128.7 (4)
O23—Mo5—O1—Mo1	−1.3 (8)	O24—Na—O5—Mo5	51.3 (4)
O5—Mo5—O1—Mo1	−179.6 (3)	O21—Mo7—O6—Mo3	−84.8 (4)
O9—Mo5—O1—Mo1	84.9 (3)	O20—Mo7—O6—Mo3	167.4 (4)
O7—Mo5—O1—Mo1	−84.4 (3)	O11—Mo7—O6—Mo3	38.6 (7)
O22—Mo5—O1—Mo1	−0.3 (2)	O3—Mo7—O6—Mo3	19.8 (3)
Mo4—Mo5—O1—Mo1	−103.4 (3)	O17—Mo3—O6—Mo7	72.6 (4)
Mo2—Mo5—O1—Mo1	103.9 (3)	O15—Mo3—O6—Mo7	177.3 (4)
Na—Mo5—O1—Mo1	178.9 (2)	O8—Mo3—O6—Mo7	−61.3 (8)
O22—Mo1—O1—Mo2	98.5 (3)	O3—Mo3—O6—Mo7	−20.0 (3)
O4—Mo1—O1—Mo2	−4.4 (3)	O2—Mo3—O6—Mo7	−93.0 (3)
O2—Mo1—O1—Mo2	−158.6 (3)	O23—Mo5—O7—Mo4	−173.2 (4)
O3—Mo1—O1—Mo2	−81.5 (3)	O5—Mo5—O7—Mo4	78.6 (4)
O22—Mo1—O1—Mo4	−97.2 (3)	O9—Mo5—O7—Mo4	−41.2 (7)
O4—Mo1—O1—Mo4	159.9 (3)	O1—Mo5—O7—Mo4	−22.1 (3)
O2—Mo1—O1—Mo4	5.7 (3)	O22—Mo5—O7—Mo4	−94.5 (3)
O3—Mo1—O1—Mo4	82.8 (3)	O14—Mo4—O7—Mo5	−173.9 (4)
O4—Mo1—O1—Mo5	−102.4 (3)	O24—Mo4—O7—Mo5	−66.8 (4)
O2—Mo1—O1—Mo5	103.4 (3)	O8—Mo4—O7—Mo5	65.4 (7)
O3—Mo1—O1—Mo5	−179.5 (3)	O1—Mo4—O7—Mo5	22.2 (3)
O16—Mo1—O2—Mo4	−176.3 (3)	O2—Mo4—O7—Mo5	94.6 (3)
O22—Mo1—O2—Mo4	75.2 (4)	O17—Mo3—O8—Mo4	173.8 (4)
O4—Mo1—O2—Mo4	−50.1 (6)	O15—Mo3—O8—Mo4	67.8 (4)
O1—Mo1—O2—Mo4	−5.6 (3)	O6—Mo3—O8—Mo4	−52.1 (8)
O3—Mo1—O2—Mo4	−96.1 (3)	O3—Mo3—O8—Mo4	−91.3 (4)
O16—Mo1—O2—Mo3	−76.2 (4)	O2—Mo3—O8—Mo4	−19.0 (3)
O22—Mo1—O2—Mo3	175.4 (3)	O14—Mo4—O8—Mo3	−69.8 (4)
O4—Mo1—O2—Mo3	50.1 (6)	O24—Mo4—O8—Mo3	−177.7 (4)
O1—Mo1—O2—Mo3	94.6 (3)	O7—Mo4—O8—Mo3	49.5 (7)
O3—Mo1—O2—Mo3	4.1 (3)	O1—Mo4—O8—Mo3	90.7 (4)
O14—Mo4—O2—Mo1	−162.4 (4)	O2—Mo4—O8—Mo3	19.1 (3)
O24—Mo4—O2—Mo1	35.8 (10)	O23—Mo5—O9—Mo2	172.7 (3)
O8—Mo4—O2—Mo1	97.5 (3)	O5—Mo5—O9—Mo2	−78.8 (4)
O7—Mo4—O2—Mo1	−69.1 (3)	O7—Mo5—O9—Mo2	41.0 (7)
O1—Mo4—O2—Mo1	6.1 (3)	O1—Mo5—O9—Mo2	21.8 (3)
O14—Mo4—O2—Mo3	86.0 (3)	O22—Mo5—O9—Mo2	94.0 (3)
O24—Mo4—O2—Mo3	−75.9 (9)	O10—Mo2—O9—Mo5	175.0 (4)

O8—Mo4—O2—Mo3	−14.2 (2)	O18—Mo2—O9—Mo5	69.1 (4)
O7—Mo4—O2—Mo3	179.3 (3)	O13—Mo2—O9—Mo5	−69.3 (7)
O1—Mo4—O2—Mo3	−105.6 (3)	O1—Mo2—O9—Mo5	−22.1 (3)
O17—Mo3—O2—Mo1	−40.2 (13)	O4—Mo2—O9—Mo5	−94.4 (3)
O15—Mo3—O2—Mo1	161.3 (4)	O21—Mo7—O11—Mo6	83.0 (4)
O8—Mo3—O2—Mo1	−98.0 (3)	O20—Mo7—O11—Mo6	−169.8 (4)
O6—Mo3—O2—Mo1	68.9 (3)	O6—Mo7—O11—Mo6	−40.1 (7)
O3—Mo3—O2—Mo1	−4.5 (3)	O3—Mo7—O11—Mo6	−21.3 (3)
O17—Mo3—O2—Mo4	72.3 (13)	O19—Mo6—O11—Mo7	−70.7 (4)
O15—Mo3—O2—Mo4	−86.3 (3)	O12—Mo6—O11—Mo7	−176.6 (4)
O8—Mo3—O2—Mo4	14.5 (2)	O13—Mo6—O11—Mo7	60.0 (8)
O6—Mo3—O2—Mo4	−178.6 (3)	O3—Mo6—O11—Mo7	21.4 (3)
O3—Mo3—O2—Mo4	108.0 (3)	O4—Mo6—O11—Mo7	94.2 (4)
O17—Mo3—O3—Mo7	−81.0 (3)	O10—Mo2—O13—Mo6	69.2 (4)
O15—Mo3—O3—Mo7	67.6 (8)	O18—Mo2—O13—Mo6	176.4 (4)
O8—Mo3—O3—Mo7	−179.1 (3)	O9—Mo2—O13—Mo6	−44.9 (8)
O6—Mo3—O3—Mo7	16.7 (3)	O1—Mo2—O13—Mo6	−89.6 (4)
O2—Mo3—O3—Mo7	107.7 (3)	O4—Mo2—O13—Mo6	−18.9 (3)
O17—Mo3—O3—Mo6	35.3 (7)	O19—Mo6—O13—Mo2	−174.1 (4)
O15—Mo3—O3—Mo6	−176.0 (7)	O12—Mo6—O13—Mo2	−67.7 (4)
O8—Mo3—O3—Mo6	−62.7 (7)	O11—Mo6—O13—Mo2	54.7 (8)
O6—Mo3—O3—Mo6	133.1 (7)	O3—Mo6—O13—Mo2	91.3 (3)
O2—Mo3—O3—Mo6	−135.9 (7)	O4—Mo6—O13—Mo2	19.2 (3)
O17—Mo3—O3—Mo1	174.9 (3)	O17—Mo3—O15—Co	−35.9 (13)
O15—Mo3—O3—Mo1	−36.5 (9)	O8—Mo3—O15—Co	65.3 (13)
O8—Mo3—O3—Mo1	76.8 (3)	O6—Mo3—O15—Co	−135.6 (13)
O6—Mo3—O3—Mo1	−87.4 (3)	O3—Mo3—O15—Co	176.4 (8)
O2—Mo3—O3—Mo1	3.6 (2)	O2—Mo3—O15—Co	138.5 (13)
O21—Mo7—O3—Mo3	77.5 (4)	OW3—Co—O15—Mo3	−49.1 (13)
O20—Mo7—O3—Mo3	−105.7 (6)	OW4—Co—O15—Mo3	43.9 (13)
O11—Mo7—O3—Mo3	173.4 (3)	OW1—Co—O15—Mo3	130.2 (13)
O6—Mo7—O3—Mo3	−17.2 (3)	OW2—Co—O15—Mo3	−139.3 (13)
O21—Mo7—O3—Mo6	−77.6 (3)	O10—Mo2—O18—Na	−150.1 (5)
O20—Mo7—O3—Mo6	99.1 (6)	O13—Mo2—O18—Na	107.5 (5)
O11—Mo7—O3—Mo6	18.3 (3)	O9—Mo2—O18—Na	−54.8 (5)
O6—Mo7—O3—Mo6	−172.3 (3)	O1—Mo2—O18—Na	19.2 (5)
O21—Mo7—O3—Mo1	−179.7 (3)	O4—Mo2—O18—Na	46.4 (13)
O20—Mo7—O3—Mo1	−2.9 (7)	O5—Na—O18—Mo2	38.4 (5)
O11—Mo7—O3—Mo1	−83.8 (3)	O5^{i}—Na—O18—Mo2	−141.6 (5)
O6—Mo7—O3—Mo1	85.6 (3)	O24^{i}—Na—O18—Mo2	140.0 (6)
O19—Mo6—O3—Mo3	−35.6 (7)	O24—Na—O18—Mo2	−40.0 (6)
O12—Mo6—O3—Mo3	170.5 (7)	O16—Mo1—O22—Mo5	−179.1 (3)
O13—Mo6—O3—Mo3	61.5 (7)	O4—Mo1—O22—Mo5	75.1 (3)
O11—Mo6—O3—Mo3	−134.2 (7)	O2—Mo1—O22—Mo5	−74.7 (3)
O4—Mo6—O3—Mo3	135.9 (7)	O1—Mo1—O22—Mo5	−0.4 (3)
Mo7—Mo6—O3—Mo3	−116.5 (8)	O23—Mo5—O22—Mo1	−180.0 (4)
O19—Mo6—O3—Mo7	80.9 (3)	O9—Mo5—O22—Mo1	−76.3 (3)
O12—Mo6—O3—Mo7	−73.0 (8)	O7—Mo5—O22—Mo1	77.5 (3)

O13—Mo6—O3—Mo7	178.0 (3)	O1—Mo5—O22—Mo1	0.5 (3)
O11—Mo6—O3—Mo7	−17.7 (3)	O14—Mo4—O24—Na	152.4 (5)
O4—Mo6—O3—Mo7	−107.6 (3)	O8—Mo4—O24—Na	−104.6 (5)
O19—Mo6—O3—Mo1	−175.2 (3)	O7—Mo4—O24—Na	55.5 (6)
O12—Mo6—O3—Mo1	30.9 (9)	O1—Mo4—O24—Na	−18.5 (6)
O13—Mo6—O3—Mo1	−78.1 (3)	O2—Mo4—O24—Na	−46.5 (12)
O11—Mo6—O3—Mo1	86.2 (3)	O18—Na—O24—Mo4	40.2 (6)
O4—Mo6—O3—Mo1	−3.8 (2)	O18^{i}—Na—O24—Mo4	−139.8 (6)
Mo7—Mo6—O3—Mo1	103.9 (3)	O5—Na—O24—Mo4	−40.9 (5)
O16—Mo1—O3—Mo3	98.4 (3)	O5^{i}—Na—O24—Mo4	139.1 (5)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
OW1—H1···OW5	0.89	2.33	2.988 (15)	131
OW1—H2···OW8	0.85	2.14	2.827 (15)	139
OW1—H1···O20^{iii}	0.89	2.05	2.837 (12)	147
OW2—H3···OW7	0.83	1.97	2.795 (17)	170
OW2—H4···O21^{iv}	0.82	2.07	2.859 (12)	162
OW3—H5···O23^{v}	0.83	2.29	2.778 (12)	118
OW3—H5···O23^{v}	0.83	2.29	2.778 (12)	118
OW4—H8···OW1	1.01	2.15	2.879 (13)	128
OW4—H8···OW8^{iii}	1.01	2.35	2.879 (16)	112
OW4—H7···O22^{v}	0.79	2.48	2.793 (11)	106
OW5—H10···OW4	1.00	2.49	3.029 (16)	114
OW5—H9···O20^{iv}	0.89	2.04	2.849 (15)	150
OW6—H11···O6	0.81	2.35	2.993 (14)	136
OW6—H12···OW7^{iii}	0.88	2.42	3.123 (17)	136
OW7—H13···O2	0.87	2.02	2.767 (13)	144
OW7—H14···OW9	0.92	2.10	2.98 (2)	161
OW8—H16···O6	0.83	2.50	2.791 (13)	102
OW8—H16···O6	0.83	2.50	2.791 (13)	102
OW8—H16···OW7	0.83	2.28	2.965 (19)	140
OW9—H17···OW6^{vi}	1.00	2.22	3.00 (2)	134
OW9—H18···OW2^{vii}	1.00	2.30	3.111 (18)	137
N1—H1A···O8	0.86	2.22	2.968 (11)	145
N1—H1B···O10^{viii}	0.86	2.14	2.967 (11)	161
N2—H2A···O9^{v}	0.86	2.18	2.992 (11)	157
N2—H2B···O8	0.86	2.18	2.936 (11)	147
N3—H3A···O9^{v}	0.86	2.48	3.216 (11)	144
N3—H3A···O10^{v}	0.86	2.28	3.031 (11)	145
N3—H3B···O13^{viii}	0.86	2.35	3.128 (11)	151
N4—H4B···O5^{ix}	0.86	2.31	2.954 (12)	131
N4—H4A···O12	0.86	2.09	2.918 (12)	160

N5—H5A···O4	0.86	2.11	2.965 (11)	177
N5—H5B···O17^{x}	0.86	2.18	3.011 (12)	161
N6—H6A···O19^{x}	0.86	2.37	2.864 (12)	117
N7—H7B···O7	0.86	2.42	3.175 (13)	147
N7—H7B···O14	0.86	2.37	3.107 (13)	144
N8—H8A···O16^{xi}	0.86	2.16	2.952 (13)	153
N8—H8B···OW6^{iv}	0.86	2.18	2.992 (18)	157
N9—H9A···O11^{xi}	0.86	2.09	2.918 (14)	162
N9—H9B···O7	0.86	2.18	2.992 (13)	157
N10—H10A···O12^{xi}	0.86	2.26	3.100 (13)	167
N10—H10B···O5	0.86	2.29	2.960 (12)	135
N11—H11B···O24^{x}	0.86	2.22	2.935 (15)	141
N11—H11A···O19^{xi}	0.86	2.09	2.916 (16)	160

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

Fig. 1

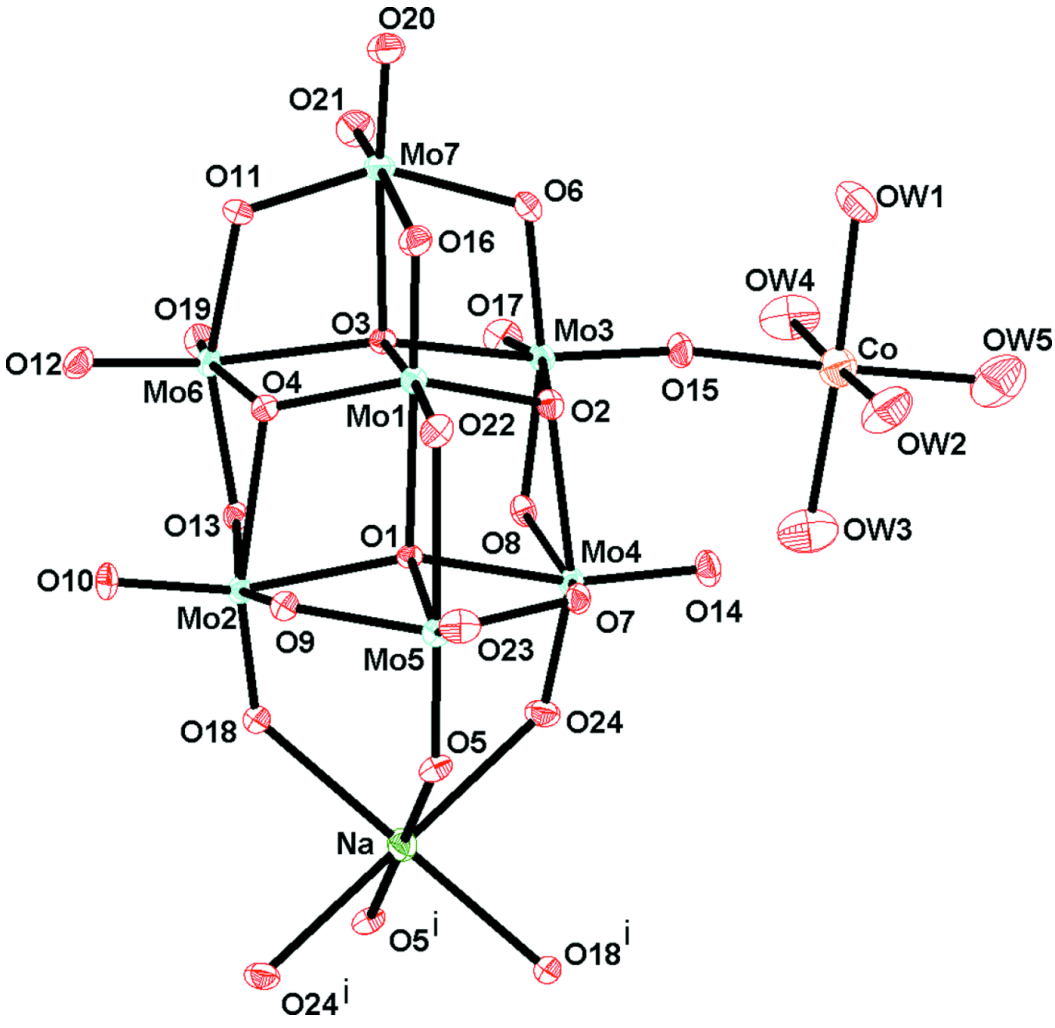
O20
O21
Mo7
O11
O6
OW1
O16
OW4
O19
O17
O3
Mo3
Co
OW5
O12
Mo6
O4
Mo1
O22
O2
O15
OW2
O13
O1
O8
Mo4
OW3
O10
Mo2
O9
Mo5
O23
O7
O14
O18
O5
O24
Na
O5i
O18i
O24i

Fig. 2