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Tetrakis(benzyltriethylammonium) octamolybdate

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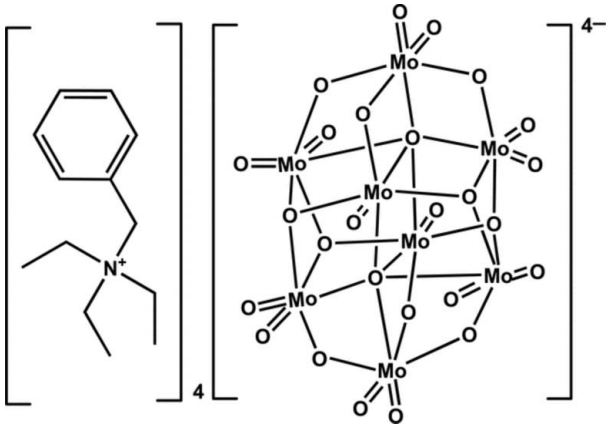
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.018 Å; R factor = 0.082; wR factor = 0.141; data-to-parameter ratio = 14.6.

The asymmetric unit of the title compound, $(C_{13}H_{22}N)_4[Mo_8O_{26}]$, comprises four independent benzyltriethylammonium cations and two independent Mo_4O_{13} units. These latter units lie about inversion centres which generate two complete $Mo_8O_{26}^{4-}$ anions in the β-isomeric form. Four discrete sets of Mo—O bond distances are found in the octamolybdate anions corresponding to terminal and μ2-, μ3- or μ5-bridging situations. In the crystal structure, an extensive array of weak intermolecular C—H···O hydrogen bonds stabilizes the crystal packing.

Related literature

For related structures, see: Wilson *et al.* (1984); Wang *et al.* (1993); Deng *et al.* (2005), Guo *et al.* (2007). For catalysis by tetra-alkylpyridinium octamolybdate compounds, see: Guo & Li (2007).



Experimental

Crystal data

$(C_{13}H_{22}N)_4[Mo_8O_{26}]$
M_r = 1952.78
Monoclinic, $P2_1/c$
a = 22.608 (5) Å
b = 18.064 (4) Å
c = 17.097 (3) Å
β = 105.54 (3)°
V = 6727 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.52 mm^{-1}
T = 294 (2) K
0.14 × 0.12 × 0.12 mm

Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.806, T_{max} = 0.835
50289 measured reflections
11863 independent reflections
8783 reflections with $I > 2\sigma(I)$
R_{int} = 0.097

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.082
$wR(F^2)$ = 0.141
S = 1.22
11863 reflections
811 parameters
30 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mo1—O7	1.694 (7)	Mo5—O15	1.671 (8)
Mo1—O1	1.698 (7)	Mo6—O19	1.700 (7)
Mo3—O4	1.698 (7)	Mo6—O17	1.720 (8)
Mo3—O9	1.700 (7)	Mo7—O20	1.694 (8)
Mo4—O5	1.712 (7)	Mo7—O23	1.720 (8)
Mo4—O10	1.715 (7)	Mo8—O16	1.695 (9)
Mo2—O6	1.696 (7)	Mo8—O26	1.704 (8)
Mo1—O12	1.891 (7)	Mo5—O21	1.775 (8)
Mo2—O13	1.754 (7)	Mo6—O22	1.889 (8)
Mo3—O3	1.917 (7)	Mo7—O22^{ii}	1.930 (8)
Mo4—O12^{i}	1.927 (7)	Mo7—O18	1.944 (7)
Mo4—O3	1.930 (7)	Mo7—O21	2.264 (8)
Mo4—O13	2.295 (7)	Mo8—O18	1.875 (8)
Mo2—O11^{i}	1.951 (7)	Mo5—O14	1.981 (7)
Mo3—O11	1.986 (7)	Mo6—O14	1.994 (7)
Mo1—O11	2.389 (7)	Mo8—O14	2.353 (8)
Mo1—O2	1.984 (6)	Mo5—O24	1.961 (7)
Mo2—O2	1.961 (7)	Mo6—O24^{ii}	2.351 (8)
Mo3—O2	2.335 (7)	Mo8—O24^{ii}	2.011 (8)
Mo1—O8	2.358 (7)	Mo5—O25	2.106 (7)
Mo2—O8	2.145 (6)	Mo5—O25^{ii}	2.415 (8)
Mo2—O8^{i}	2.406 (7)	Mo6—O25	2.347 (7)
Mo3—O8^{i}	2.334 (7)	Mo7—O25^{ii}	2.446 (8)
Mo4—O8^{i}	2.445 (6)	Mo8—O25^{ii}	2.389 (7)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C49—H49A···O19^{iii}	0.97	2.59	3.371 (15)	138
C46—H46B···O21^{iv}	0.97	2.60	3.098 (13)	112
C38—H38B···O12^{v}	0.97	2.56	3.508 (14)	166
C37—H37A···O12^{v}	0.96	2.29	3.199 (13)	157
C36—H36B···O6	0.97	2.45	3.144 (13)	128
C36—H36B···O1	0.97	2.54	3.381 (14)	146
C33—H33A···O1	0.97	2.29	3.212 (12)	158
C29—H29···O5^{vi}	0.93	2.48	3.177 (15)	132
C26—H26A···O23^{vii}	0.96	2.55	3.219 (15)	127
C25—H25A···O2^{vii}	0.97	2.37	3.037 (12)	126
C24—H24C···O4^{vii}	0.96	2.56	3.464 (16)	158
C23—H23A···O17^{viii}	0.97	2.40	3.360 (14)	169
C22—H22C···O20	0.96	2.59	3.326 (16)	134

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D—H···A	D—H	H···A	D···A	D—H···A
C21—H21A···O3^{vii}	0.97	2.57	3.499 (14)	160
C18—H18···O20	0.93	2.48	3.370 (15)	160
C12—H12A···O4^{vi}	0.97	2.44	3.182 (13)	133
C10—H10B···O7^{ix}	0.97	2.50	3.320 (15)	142
C9—H9B···O17^{x}	0.96	2.42	3.209 (14)	139
C8—H8A···O16^{ix}	0.97	2.42	3.339 (15)	158
C7—H7A···O7^{ix}	0.97	2.40	3.221 (13)	142
C5—H5···O3^{vi}	0.93	2.49	3.320 (13)	149

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: SJ2287).

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supplementary materials

Acta Cryst. (2007). E**63**, m1456-m1457 [**doi:10.1107/S1600536807018351**]

Tetrakis(benzyltriethylammonium) octamolybdate

M.-L. Guo, C.-H. Guo, H.-Z. Li and H. Chang

Comment

Some tetra-alkylpyridinium octamolybdate compounds were found to be efficient catalysts for the selective oxidation of benzyl alcohol with aqueous hydrogen peroxide (Guo and Li, 2007). We have recently reported the crystal structure of tetra-hexylpyridinium octamolybdate (Guo *et al.*, 2007). The present crystal structure of the related octamolybdate salt (I), is part of this study.

The asymmetric unit in the structure of (I) comprises two nonequivalent Mo_4O_{13} motifs and four nonequivalent benzyltriethylammonium cations, and a symmetry-expanded view, Fig 1, displays the two complete $Mo_8O_{26}^{4-}$ anions in the β-isomeric form. The structure of the anions, as described recently (Guo and Li, 2007), is constructed from an array of eight edge-shared MoO_6 octahedra. The Mo–O distances are significantly different, ranging from 1.671 (8) to 2.446 (8) Å, and can be grouped into four sets: Mo–O(terminal) 1.671 (8)–1.720 (8)Å and Mo–O(μ2) 1.754 (7)–2.295 (7) Å, Mo–O(μ3) 1.951 (7)—2.353 (8) Å, Mo–O(μ5) 2.106 (7)– 2.446 (8)Å bridging groups, Table 1.

In the crystal structure of (I), no classical hydrogen bonds are found, but an extensive array of weak C–H···O interactions (Table 2) stabilise the structure in a three-dimensional network, Fig. 2.

Experimental

A solution of benzyltriethylammonium chloride (1.9 g, 8 mmol) in 10 ml of distilled water was added dropwise into a mixture of 20 ml aqueous solution of sodium molybdate dihydrate (1.2 g, 5 mmol) and 12% dilute hydrogen chloride

(1.8 ml, 7 mmol) with stirring at 70°C. A white precipitate was immediately formed. After stirring continuously for 20 min, the resulting product was filtered, washed with water and dried at room temperature to produce the tetrakis(benzyltriethylammonium) octamolybdate in 81% yield. Single crystals were grown in the filtrate by slow evaporation over a period of 2 d at 30°C.

Refinement

The H atoms bonded to C atoms were included in the refinement in the riding model approximation, with C–H = 0.93–0.97 Å and U_{iso} (H) = 1.2 U_{eq} (C atom). For the H atoms attached to C atoms of methyl groups, their U_{iso}(H) = 1.5U_{eq}(C).

Figures

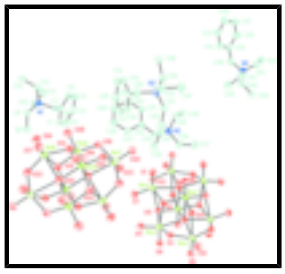

Fig. 1. A view of the structure of (I), showing the atom-numbering Scheme; displacement ellipsoids were drawn at the 30% probability level. The unlabelled atoms in the Mo1···Mo4 β-octamolybdate are related to the labelled atoms by the symmetry operator x+1, y+1, -z, while those of the second β- octamolybdate are related by x+2, y+1, z+1.

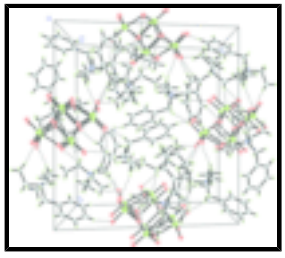

Fig. 2. The crystal packing of (I) viewed down the a axis with hydrogen bonds drawn as dashed lines.

Tetrakis(benzyltriethylammonium) octamolybdate

Crystal data

$(C_{13}H_{22}N)_4[Mo_8O_{26}]$	F_{000} = 3888
M_r = 1952.78	D_x = 1.928 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 11210 reflections
a = 22.608 (5) Å	θ = 1.5–27.9º
b = 18.064 (4) Å	μ = 1.52 mm^{-1}
c = 17.097 (3) Å	T = 294 (2) K
β = 105.54 (3)º	Block, colorless
V = 6727 (3) Å^3	0.14 × 0.12 × 0.12 mm
Z = 4	

Data collection

Rigaku Saturn diffractometer	11863 independent reflections
Radiation source: fine-focus sealed tube	8783 reflections with $I > 2\sigma(I)$
Monochromator: confocal	R_{int} = 0.097
T = 294(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (Jacobson, 1998)	h = −26→26
T_{min} = 0.806, T_{max} = 0.835	k = −21→21
50289 measured reflections	l = −20→20

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.082$	$w = 1/[\sigma^2(F_o^2) + (0.0201P)^2 + 8.4317P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.141$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.22$	$\Delta\rho_{max} = 0.52$ e Å^{-3}
11863 reflections	$\Delta\rho_{min} = -0.66$ e Å^{-3}
811 parameters	Extinction correction: none
30 restraints	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

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.

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}
Mo1	0.56189 (5)	0.44651 (5)	0.16037 (6)	0.0529 (2)
Mo2	0.54754 (5)	0.58013 (5)	0.03087 (6)	0.0515 (2)
Mo3	0.59708 (5)	0.40315 (5)	−0.01661 (6)	0.0538 (2)
Mo4	0.58509 (5)	0.53700 (5)	−0.14789 (6)	0.0551 (3)
Mo5	1.01867 (5)	0.59332 (6)	0.52890 (6)	0.0596 (3)
Mo6	1.05392 (5)	0.47011 (6)	0.67075 (6)	0.0580 (3)
Mo7	0.86154 (5)	0.61037 (6)	0.43350 (7)	0.0657 (3)
Mo8	0.89988 (5)	0.48503 (6)	0.57679 (7)	0.0639 (3)
O1	0.5826 (3)	0.5119 (4)	0.2340 (4)	0.0604 (19)
O2	0.5980 (3)	0.4951 (4)	0.0797 (4)	0.0503 (17)
O3	0.6375 (3)	0.4779 (4)	−0.0630 (4)	0.0539 (18)
O4	0.6583 (3)	0.3641 (4)	0.0507 (4)	0.0582 (19)
O5	0.5665 (3)	0.4697 (4)	−0.2209 (4)	0.0592 (19)
O6	0.5674 (3)	0.6422 (4)	0.1079 (4)	0.0580 (19)
O7	0.6122 (3)	0.3764 (4)	0.1933 (4)	0.0573 (19)
O8	0.4826 (3)	0.5142 (4)	0.0714 (4)	0.0501 (17)

O9	0.5779 (3)	0.3422 (4)	−0.0951 (4)	0.0549 (18)
O10	0.6372 (3)	0.5929 (4)	−0.1761 (4)	0.063 (2)
O11	0.5303 (3)	0.3804 (3)	0.0350 (4)	0.0505 (17)
O12	0.4897 (3)	0.4062 (4)	0.1791 (4)	0.0535 (18)
O13	0.5919 (3)	0.6074 (4)	−0.0340 (4)	0.0542 (18)
O14	0.9937 (3)	0.5488 (4)	0.6210 (4)	0.062 (2)
O15	1.0765 (4)	0.6478 (4)	0.5779 (5)	0.064 (2)
O16	0.8417 (4)	0.4290 (5)	0.5273 (5)	0.082 (3)
O17	1.1122 (4)	0.5291 (4)	0.7184 (5)	0.069 (2)
O18	0.8692 (4)	0.5800 (4)	0.5449 (4)	0.064 (2)
O19	1.0259 (4)	0.4401 (4)	0.7480 (5)	0.075 (2)
O20	0.8310 (4)	0.6964 (5)	0.4285 (5)	0.078 (2)
O21	0.9553 (4)	0.6548 (4)	0.4992 (4)	0.062 (2)
O22	1.0992 (4)	0.3865 (4)	0.6537 (5)	0.068 (2)
O23	0.8006 (4)	0.5544 (5)	0.3875 (5)	0.079 (2)
O24	1.0311 (4)	0.5860 (4)	0.4200 (4)	0.062 (2)
O25	1.0628 (4)	0.4897 (4)	0.5387 (5)	0.065 (2)
O26	0.8971 (4)	0.4826 (4)	0.6753 (5)	0.073 (2)
N1	0.7180 (4)	0.2127 (5)	0.8806 (5)	0.056 (2)
C1	0.7560 (5)	0.3185 (7)	0.7358 (7)	0.062 (3)
H1	0.7620	0.2724	0.7148	0.074*
C2	0.7852 (5)	0.3788 (7)	0.7155 (7)	0.065 (3)
H2	0.8115	0.3731	0.6824	0.078*
C3	0.7757 (5)	0.4484 (7)	0.7439 (7)	0.064 (3)
H3	0.7954	0.4897	0.7302	0.077*
C4	0.7364 (5)	0.4552 (6)	0.7929 (7)	0.062 (3)
H4	0.7291	0.5017	0.8118	0.074*
C5	0.7076 (5)	0.3931 (6)	0.8144 (7)	0.060 (3)
H5	0.6813	0.3986	0.8477	0.072*
C6	0.7176 (5)	0.3238 (6)	0.7870 (7)	0.055 (3)
C7	0.6846 (5)	0.2561 (6)	0.8050 (6)	0.053 (3)
H7A	0.6772	0.2232	0.7585	0.064*
H7B	0.6449	0.2713	0.8111	0.064*
C8	0.7806 (5)	0.1864 (7)	0.8745 (7)	0.066 (3)
H8A	0.8028	0.1653	0.9262	0.079*
H8B	0.8037	0.2288	0.8641	0.079*
C9	0.7770 (6)	0.1287 (7)	0.8076 (7)	0.068 (3)
H9A	0.7658	0.0816	0.8252	0.103*
H9B	0.8163	0.1247	0.7964	0.103*
H9C	0.7468	0.1437	0.7592	0.103*
C10	0.6798 (6)	0.1457 (6)	0.8898 (8)	0.066 (3)
H10A	0.7038	0.1146	0.9330	0.080*
H10B	0.6709	0.1171	0.8399	0.080*
C11	0.6190 (6)	0.1653 (7)	0.9087 (9)	0.083 (4)
H11A	0.6274	0.1860	0.9622	0.125*
H11B	0.5946	0.1214	0.9058	0.125*
H11C	0.5971	0.2008	0.8698	0.125*
C12	0.7293 (6)	0.2634 (6)	0.9527 (7)	0.060 (3)
H12A	0.6908	0.2876	0.9522	0.072*

H12B	0.7577	0.3017	0.9462	0.072*
C13	0.7545 (6)	0.2283 (7)	1.0353 (7)	0.072 (3)
H13A	0.7283	0.1883	1.0417	0.108*
H13B	0.7563	0.2646	1.0768	0.108*
H13C	0.7950	0.2096	1.0396	0.108*
N2	0.7787 (4)	0.9129 (5)	0.5839 (5)	0.059 (2)
C14	0.7592 (5)	0.7746 (7)	0.7127 (7)	0.066 (3)
H14	0.7639	0.8119	0.7515	0.079*
C15	0.7270 (6)	0.7108 (8)	0.7218 (9)	0.084 (4)
H15	0.7088	0.7068	0.7644	0.101*
C16	0.7224 (6)	0.6529 (7)	0.6666 (9)	0.081 (4)
H16	0.7021	0.6095	0.6729	0.097*
C17	0.7482 (6)	0.6608 (8)	0.6025 (8)	0.078 (4)
H17	0.7455	0.6222	0.5657	0.094*
C18	0.7780 (6)	0.7254 (7)	0.5924 (7)	0.069 (3)
H18	0.7942	0.7301	0.5481	0.083*
C19	0.7843 (6)	0.7843 (7)	0.6479 (7)	0.071 (3)
C20	0.8178 (6)	0.8533 (6)	0.6373 (8)	0.069 (3)
H20A	0.8510	0.8400	0.6140	0.082*
H20B	0.8361	0.8743	0.6905	0.082*
C21	0.7529 (6)	0.8885 (7)	0.4962 (7)	0.068 (3)
H21A	0.7247	0.9262	0.4678	0.082*
H21B	0.7296	0.8433	0.4956	0.082*
C22	0.8016 (6)	0.8747 (8)	0.4493 (8)	0.081 (4)
H22A	0.8272	0.9177	0.4531	0.122*
H22B	0.7814	0.8649	0.3933	0.122*
H22C	0.8264	0.8329	0.4723	0.122*
C23	0.8199 (6)	0.9804 (7)	0.5888 (7)	0.069 (3)
H23A	0.8341	0.9954	0.6453	0.082*
H23B	0.8557	0.9657	0.5716	0.082*
C24	0.7915 (6)	1.0469 (7)	0.5394 (8)	0.082 (4)
H24A	0.7809	1.0345	0.4827	0.123*
H24B	0.8203	1.0871	0.5496	0.123*
H24C	0.7551	1.0613	0.5543	0.123*
C25	0.7233 (5)	0.9319 (7)	0.6148 (7)	0.063 (3)
H25A	0.6965	0.9640	0.5753	0.075*
H25B	0.7010	0.8866	0.6174	0.075*
C26	0.7370 (6)	0.9693 (7)	0.6969 (7)	0.077 (4)
H26A	0.7724	0.9468	0.7328	0.115*
H26B	0.7024	0.9639	0.7189	0.115*
H26C	0.7448	1.0209	0.6909	0.115*
N3	0.5509 (4)	0.6765 (5)	0.3595 (5)	0.057 (2)
C27	0.6186 (6)	0.5264 (6)	0.4861 (7)	0.064 (3)
H27	0.6398	0.5173	0.4474	0.077*
C28	0.6399 (6)	0.4942 (6)	0.5636 (8)	0.072 (3)
H28	0.6740	0.4633	0.5763	0.086*
C29	0.6076 (6)	0.5105 (7)	0.6207 (8)	0.075 (4)
H29	0.6207	0.4901	0.6724	0.090*
C30	0.5579 (6)	0.5551 (7)	0.6024 (7)	0.068 (3)

H30	0.5376	0.5655	0.6418	0.082*
C31	0.5368 (6)	0.5853 (7)	0.5256 (7)	0.067 (3)
H31	0.5022	0.6154	0.5135	0.080*
C32	0.5673 (6)	0.5709 (6)	0.4661 (7)	0.060 (3)
C33	0.5445 (6)	0.5960 (6)	0.3787 (6)	0.059 (3)
H33A	0.5659	0.5672	0.3469	0.071*
H33B	0.5013	0.5832	0.3597	0.071*
C34	0.6175 (6)	0.7015 (7)	0.3929 (7)	0.069 (3)
H34A	0.6197	0.7544	0.3845	0.083*
H34B	0.6299	0.6927	0.4510	0.083*
C35	0.6629 (6)	0.6630 (7)	0.3549 (8)	0.076 (4)
H35A	0.6613	0.6105	0.3630	0.114*
H35B	0.7036	0.6806	0.3799	0.114*
H35C	0.6524	0.6735	0.2978	0.114*
C36	0.5300 (6)	0.6809 (6)	0.2675 (7)	0.066 (3)
H36A	0.4876	0.6647	0.2496	0.079*
H36B	0.5543	0.6466	0.2455	0.079*
C37	0.5348 (6)	0.7582 (6)	0.2317 (7)	0.070 (3)
H37A	0.5180	0.7945	0.2607	0.105*
H37B	0.5124	0.7588	0.1754	0.105*
H37C	0.5772	0.7695	0.2367	0.105*
C38	0.5121 (6)	0.7261 (7)	0.3982 (7)	0.069 (3)
H38A	0.5271	0.7216	0.4567	0.083*
H38B	0.5181	0.7770	0.3842	0.083*
C39	0.4447 (6)	0.7103 (7)	0.3744 (8)	0.072 (3)
H39A	0.4300	0.7088	0.3163	0.108*
H39B	0.4236	0.7485	0.3952	0.108*
H39C	0.4373	0.6634	0.3965	0.108*
N4	−0.0084 (5)	0.8058 (6)	0.3114 (6)	0.0695 (18)
C40	−0.0182 (7)	0.8699 (9)	0.4980 (9)	0.095 (5)
H40	−0.0597	0.8717	0.4707	0.115*
C41	0.0038 (7)	0.9119 (9)	0.5664 (9)	0.093 (5)
H41	−0.0225	0.9440	0.5832	0.111*
C42	0.0637 (7)	0.9070 (8)	0.6102 (9)	0.088 (4)
H42	0.0778	0.9329	0.6587	0.106*
C43	0.1027 (7)	0.8634 (8)	0.5814 (8)	0.089 (4)
H43	0.1440	0.8610	0.6096	0.107*
C44	0.0812 (7)	0.8226 (8)	0.5105 (8)	0.084 (4)
H44	0.1085	0.7937	0.4915	0.100*
C45	0.0213 (6)	0.8244 (7)	0.4687 (7)	0.068 (3)
C46	−0.0047 (6)	0.7750 (7)	0.3945 (7)	0.069 (2)
H46A	0.0201	0.7304	0.4013	0.083*
H46B	−0.0458	0.7602	0.3954	0.083*
C47	0.0539 (6)	0.8279 (7)	0.3035 (8)	0.077 (2)
H47A	0.0723	0.8622	0.3467	0.092*
H47B	0.0489	0.8535	0.2522	0.092*
C48	0.0979 (7)	0.7617 (8)	0.3071 (9)	0.096 (4)
H48A	0.0993	0.7325	0.3545	0.145*
H48B	0.1383	0.7798	0.3096	0.145*

H48C	0.0835	0.7317	0.2594	0.145*
C49	−0.0362 (6)	0.7461 (7)	0.2506 (7)	0.075 (3)
H49A	−0.0108	0.7021	0.2632	0.090*
H49B	−0.0764	0.7337	0.2567	0.090*
C50	−0.0427 (6)	0.7669 (7)	0.1634 (7)	0.079 (4)
H50A	−0.0713	0.8070	0.1483	0.118*
H50B	−0.0573	0.7250	0.1291	0.118*
H50C	−0.0035	0.7819	0.1571	0.118*
C51	−0.0456 (6)	0.8748 (7)	0.2956 (8)	0.073 (3)
H51A	−0.0414	0.8964	0.2454	0.088*
H51B	−0.0284	0.9097	0.3388	0.088*
C52	−0.1146 (6)	0.8662 (9)	0.2889 (9)	0.095 (5)
H52A	−0.1342	0.8405	0.2396	0.143*
H52B	−0.1328	0.9143	0.2884	0.143*
H52C	−0.1197	0.8385	0.3345	0.143*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.0576 (6)	0.0534 (5)	0.0480 (6)	0.0019 (5)	0.0147 (5)	0.0013 (4)
Mo2	0.0550 (6)	0.0494 (5)	0.0509 (6)	0.0004 (4)	0.0158 (5)	−0.0005 (4)
Mo3	0.0581 (6)	0.0520 (5)	0.0533 (6)	0.0035 (5)	0.0184 (5)	0.0005 (4)
Mo4	0.0593 (6)	0.0565 (6)	0.0513 (6)	0.0023 (5)	0.0180 (5)	0.0003 (4)
Mo5	0.0705 (7)	0.0548 (6)	0.0545 (6)	−0.0034 (5)	0.0186 (5)	0.0012 (5)
Mo6	0.0619 (6)	0.0590 (6)	0.0538 (6)	0.0013 (5)	0.0167 (5)	0.0028 (5)
Mo7	0.0683 (7)	0.0684 (7)	0.0607 (7)	0.0075 (6)	0.0176 (6)	−0.0011 (5)
Mo8	0.0675 (7)	0.0629 (6)	0.0657 (7)	−0.0041 (5)	0.0256 (6)	−0.0013 (5)
O1	0.066 (5)	0.066 (5)	0.052 (5)	−0.001 (4)	0.021 (4)	0.000 (4)
O2	0.054 (4)	0.048 (4)	0.048 (4)	−0.001 (3)	0.013 (3)	0.006 (3)
O3	0.060 (5)	0.052 (4)	0.052 (4)	0.002 (3)	0.021 (4)	0.001 (3)
O4	0.062 (5)	0.055 (4)	0.061 (5)	0.005 (4)	0.022 (4)	0.000 (4)
O5	0.065 (5)	0.057 (4)	0.054 (5)	0.007 (4)	0.014 (4)	−0.007 (3)
O6	0.068 (5)	0.048 (4)	0.057 (5)	0.001 (4)	0.016 (4)	−0.002 (3)
O7	0.058 (5)	0.056 (4)	0.059 (5)	0.003 (4)	0.017 (4)	0.004 (3)
O8	0.053 (4)	0.053 (4)	0.048 (4)	0.000 (3)	0.018 (3)	0.002 (3)
O9	0.053 (5)	0.054 (4)	0.056 (5)	0.000 (3)	0.012 (4)	−0.005 (3)
O10	0.065 (5)	0.067 (5)	0.061 (5)	−0.003 (4)	0.022 (4)	0.001 (4)
O11	0.058 (5)	0.044 (4)	0.050 (4)	0.001 (3)	0.015 (4)	0.001 (3)
O12	0.055 (5)	0.054 (4)	0.053 (4)	−0.001 (3)	0.018 (4)	0.005 (3)
O13	0.061 (5)	0.051 (4)	0.051 (4)	0.000 (4)	0.016 (4)	0.002 (3)
O14	0.070 (5)	0.060 (5)	0.057 (5)	0.001 (4)	0.021 (4)	0.004 (4)
O15	0.064 (5)	0.051 (4)	0.074 (5)	−0.004 (4)	0.013 (4)	0.003 (4)
O16	0.089 (7)	0.082 (6)	0.078 (6)	−0.016 (5)	0.026 (5)	−0.011 (5)
O17	0.073 (6)	0.068 (5)	0.061 (5)	0.002 (4)	0.010 (4)	0.001 (4)
O18	0.066 (5)	0.069 (5)	0.061 (5)	0.006 (4)	0.026 (4)	−0.006 (4)
O19	0.093 (7)	0.073 (5)	0.066 (5)	0.000 (5)	0.034 (5)	0.012 (4)
O20	0.086 (6)	0.087 (6)	0.064 (5)	0.027 (5)	0.024 (5)	0.008 (4)
O21	0.074 (6)	0.059 (5)	0.055 (5)	0.004 (4)	0.023 (4)	0.006 (4)

O22	0.081 (6)	0.061 (5)	0.064 (5)	0.005 (4)	0.023 (4)	0.004 (4)
O23	0.069 (6)	0.095 (7)	0.072 (6)	−0.009 (5)	0.015 (5)	−0.013 (5)
O24	0.072 (5)	0.062 (5)	0.053 (5)	0.000 (4)	0.019 (4)	0.000 (4)
O25	0.080 (6)	0.058 (5)	0.062 (5)	0.006 (4)	0.027 (4)	0.011 (4)
O26	0.079 (6)	0.069 (5)	0.075 (6)	−0.004 (4)	0.027 (5)	−0.001 (4)
N1	0.067 (6)	0.048 (5)	0.054 (6)	−0.001 (4)	0.016 (5)	−0.006 (4)
C1	0.062 (8)	0.072 (8)	0.056 (7)	−0.001 (6)	0.021 (6)	−0.010 (6)
C2	0.054 (7)	0.074 (8)	0.071 (8)	−0.005 (6)	0.024 (6)	0.000 (6)
C3	0.061 (8)	0.067 (8)	0.062 (8)	−0.013 (6)	0.011 (6)	0.004 (6)
C4	0.065 (8)	0.059 (7)	0.058 (7)	−0.004 (6)	0.010 (6)	−0.002 (5)
C5	0.054 (7)	0.067 (7)	0.059 (7)	0.009 (6)	0.015 (6)	0.006 (6)
C6	0.058 (7)	0.056 (6)	0.051 (7)	−0.003 (5)	0.013 (6)	0.000 (5)
C7	0.054 (7)	0.060 (7)	0.045 (6)	0.009 (5)	0.010 (5)	0.002 (5)
C8	0.066 (8)	0.068 (8)	0.064 (8)	0.010 (6)	0.016 (6)	−0.004 (6)
C9	0.062 (8)	0.073 (8)	0.068 (8)	0.009 (6)	0.013 (6)	−0.002 (6)
C10	0.074 (9)	0.052 (7)	0.075 (8)	−0.003 (6)	0.024 (7)	0.013 (6)
C11	0.069 (9)	0.069 (8)	0.112 (12)	0.000 (7)	0.025 (8)	0.020 (8)
C12	0.069 (8)	0.054 (6)	0.058 (7)	0.007 (6)	0.017 (6)	0.004 (5)
C13	0.088 (10)	0.070 (8)	0.061 (8)	0.013 (7)	0.026 (7)	−0.010 (6)
N2	0.062 (6)	0.058 (6)	0.053 (6)	0.003 (5)	0.011 (5)	0.005 (4)
C14	0.065 (8)	0.074 (8)	0.060 (8)	0.020 (6)	0.018 (6)	−0.002 (6)
C15	0.080 (10)	0.074 (9)	0.112 (12)	0.014 (7)	0.047 (9)	0.027 (8)
C16	0.077 (10)	0.063 (8)	0.100 (11)	−0.002 (7)	0.021 (9)	−0.002 (7)
C17	0.081 (10)	0.074 (9)	0.078 (10)	0.004 (7)	0.018 (8)	0.002 (7)
C18	0.084 (9)	0.061 (7)	0.064 (8)	0.005 (7)	0.020 (7)	0.004 (6)
C19	0.081 (9)	0.073 (8)	0.057 (8)	0.009 (7)	0.016 (7)	0.001 (6)
C20	0.060 (8)	0.064 (8)	0.079 (9)	0.004 (6)	0.012 (7)	0.002 (6)
C21	0.074 (9)	0.075 (8)	0.054 (7)	0.016 (7)	0.016 (7)	0.002 (6)
C22	0.096 (11)	0.090 (10)	0.067 (9)	0.007 (8)	0.037 (8)	−0.009 (7)
C23	0.067 (8)	0.081 (9)	0.050 (7)	−0.004 (7)	0.002 (6)	−0.009 (6)
C24	0.092 (11)	0.064 (8)	0.086 (10)	−0.003 (7)	0.017 (8)	0.010 (7)
C25	0.051 (7)	0.073 (8)	0.065 (8)	0.015 (6)	0.016 (6)	0.003 (6)
C26	0.088 (10)	0.077 (9)	0.069 (9)	0.010 (7)	0.030 (8)	−0.010 (7)
N3	0.075 (7)	0.049 (5)	0.056 (6)	−0.002 (5)	0.033 (5)	0.003 (4)
C27	0.068 (8)	0.065 (7)	0.057 (7)	−0.013 (6)	0.013 (6)	0.000 (6)
C28	0.081 (9)	0.058 (7)	0.080 (9)	0.008 (6)	0.029 (8)	−0.001 (6)
C29	0.079 (10)	0.074 (9)	0.062 (8)	−0.024 (7)	0.003 (7)	−0.007 (7)
C30	0.080 (9)	0.084 (9)	0.044 (7)	−0.004 (7)	0.021 (6)	−0.008 (6)
C31	0.070 (8)	0.079 (8)	0.057 (7)	−0.001 (6)	0.026 (7)	−0.001 (6)
C32	0.062 (8)	0.058 (7)	0.058 (7)	−0.004 (6)	0.009 (6)	0.001 (5)
C33	0.080 (8)	0.048 (6)	0.055 (7)	0.002 (6)	0.028 (6)	−0.005 (5)
C34	0.071 (9)	0.073 (8)	0.058 (8)	−0.018 (7)	0.006 (7)	0.000 (6)
C35	0.072 (9)	0.079 (9)	0.079 (9)	−0.007 (7)	0.022 (8)	0.008 (7)
C36	0.085 (9)	0.063 (7)	0.048 (7)	−0.001 (7)	0.015 (6)	−0.001 (5)
C37	0.091 (10)	0.059 (7)	0.056 (7)	0.002 (7)	0.010 (7)	0.002 (6)
C38	0.088 (10)	0.063 (7)	0.061 (8)	0.010 (7)	0.030 (7)	−0.006 (6)
C39	0.071 (9)	0.074 (8)	0.072 (9)	0.006 (7)	0.020 (7)	0.000 (6)
N4	0.070 (4)	0.073 (4)	0.067 (4)	−0.005 (3)	0.021 (4)	0.004 (3)
C40	0.070 (10)	0.134 (14)	0.087 (11)	−0.003 (9)	0.029 (8)	−0.030 (10)

C41	0.072 (10)	0.130 (13)	0.082 (10)	−0.001 (9)	0.030 (8)	−0.032 (9)
C42	0.089 (11)	0.096 (11)	0.074 (10)	−0.011 (9)	0.012 (9)	−0.012 (8)
C43	0.094 (11)	0.106 (11)	0.061 (9)	0.014 (9)	0.011 (8)	−0.010 (8)
C44	0.078 (10)	0.096 (10)	0.074 (9)	0.024 (8)	0.015 (8)	−0.007 (8)
C45	0.079 (9)	0.078 (8)	0.047 (7)	−0.010 (7)	0.017 (7)	0.010 (6)
C46	0.070 (5)	0.073 (5)	0.067 (5)	−0.009 (4)	0.022 (5)	0.006 (4)
C47	0.072 (5)	0.084 (5)	0.074 (5)	−0.001 (4)	0.018 (5)	0.003 (4)
C48	0.083 (8)	0.109 (8)	0.092 (8)	0.018 (7)	0.014 (7)	−0.003 (7)
C49	0.075 (5)	0.080 (5)	0.070 (5)	−0.005 (5)	0.019 (5)	−0.001 (4)
C50	0.083 (10)	0.089 (10)	0.064 (9)	−0.011 (8)	0.022 (7)	−0.005 (7)
C51	0.077 (5)	0.075 (5)	0.068 (5)	−0.005 (5)	0.018 (5)	0.010 (4)
C52	0.085 (11)	0.124 (13)	0.080 (10)	0.018 (9)	0.027 (9)	−0.001 (9)

Geometric parameters (Å, °)

Mo1—O7	1.694 (7)	C17—H17	0.9300
Mo1—O1	1.698 (7)	C18—C19	1.407 (16)
Mo3—O4	1.698 (7)	C18—H18	0.9300
Mo3—O9	1.700 (7)	C19—C20	1.496 (16)
Mo4—O5	1.712 (7)	C20—H20A	0.9700
Mo4—O10	1.715 (7)	C20—H20B	0.9700
Mo2—O6	1.696 (7)	C21—C22	1.546 (15)
Mo1—O12	1.891 (7)	C21—H21A	0.9700
Mo2—O13	1.754 (7)	C21—H21B	0.9700
Mo3—O3	1.917 (7)	C22—H22A	0.9600
Mo4—O12^{i}	1.927 (7)	C22—H22B	0.9600
Mo4—O3	1.930 (7)	C22—H22C	0.9600
Mo4—O13	2.295 (7)	C23—C24	1.510 (16)
Mo2—O11^{i}	1.951 (7)	C23—H23A	0.9700
Mo3—O11	1.986 (7)	C23—H23B	0.9700
Mo1—O11	2.389 (7)	C24—H24A	0.9600
Mo1—O2	1.984 (6)	C24—H24B	0.9600
Mo2—O2	1.961 (7)	C24—H24C	0.9600
Mo3—O2	2.335 (7)	C25—C26	1.513 (15)
Mo1—O8	2.358 (7)	C25—H25A	0.9700
Mo2—O8	2.145 (6)	C25—H25B	0.9700
Mo2—O8^{i}	2.406 (7)	C26—H26A	0.9600
Mo3—O8^{i}	2.334 (7)	C26—H26B	0.9600
Mo4—O8^{i}	2.445 (6)	C26—H26C	0.9600
Mo5—O15	1.671 (8)	N3—C33	1.506 (12)
Mo6—O19	1.700 (7)	N3—C36	1.519 (13)
Mo6—O17	1.720 (8)	N3—C38	1.523 (13)
Mo7—O20	1.694 (8)	N3—C34	1.529 (14)
Mo7—O23	1.720 (8)	C27—C32	1.377 (16)
Mo8—O16	1.695 (9)	C27—C28	1.408 (16)
Mo8—O26	1.704 (8)	C27—H27	0.9300
Mo5—O21	1.775 (8)	C28—C29	1.397 (17)
Mo6—O22	1.889 (8)	C28—H28	0.9300

Mo7—O22^{ii}	1.930 (8)	C29—C30	1.350 (17)
Mo7—O18	1.944 (7)	C29—H29	0.9300
Mo7—O21	2.264 (8)	C30—C31	1.384 (15)
Mo8—O18	1.875 (8)	C30—H30	0.9300
Mo5—O14	1.981 (7)	C31—C32	1.397 (15)
Mo6—O14	1.994 (7)	C31—H31	0.9300
Mo8—O14	2.353 (8)	C32—C33	1.514 (14)
Mo5—O24	1.961 (7)	C33—H33A	0.9700
Mo6—O24^{ii}	2.351 (8)	C33—H33B	0.9700
Mo8—O24^{ii}	2.011 (8)	C34—C35	1.522 (16)
Mo5—O25	2.106 (7)	C34—H34A	0.9700
Mo5—O25^{ii}	2.415 (8)	C34—H34B	0.9700
Mo6—O25	2.347 (7)	C35—H35A	0.9600
Mo7—O25^{ii}	2.446 (8)	C35—H35B	0.9600
Mo8—O25^{ii}	2.389 (7)	C35—H35C	0.9600
N1—C12	1.503 (13)	C36—C37	1.540 (15)
N1—C10	1.521 (13)	C36—H36A	0.9700
N1—C8	1.522 (14)	C36—H36B	0.9700
N1—C7	1.527 (12)	C37—H37A	0.9600
C1—C2	1.366 (15)	C37—H37B	0.9600
C1—C6	1.392 (14)	C37—H37C	0.9600
C1—H1	0.9300	C38—C39	1.494 (16)
C2—C3	1.384 (16)	C38—H38A	0.9700
C2—H2	0.9300	C38—H38B	0.9700
C3—C4	1.382 (15)	C39—H39A	0.9600
C3—H3	0.9300	C39—H39B	0.9600
C4—C5	1.395 (15)	C39—H39C	0.9600
C4—H4	0.9300	N4—C51	1.488 (15)
C5—C6	1.378 (15)	N4—C47	1.504 (15)
C5—H5	0.9300	N4—C46	1.507 (14)
C6—C7	1.507 (14)	N4—C49	1.514 (15)
C7—H7A	0.9700	C40—C41	1.370 (18)
C7—H7B	0.9700	C40—C45	1.400 (18)
C8—C9	1.534 (15)	C40—H40	0.9300
C8—H8A	0.9700	C41—C42	1.364 (18)
C8—H8B	0.9700	C41—H41	0.9300
C9—H9A	0.9600	C42—C43	1.368 (19)
C9—H9B	0.9600	C42—H42	0.9300
C9—H9C	0.9600	C43—C44	1.391 (17)
C10—C11	1.534 (16)	C43—H43	0.9300
C10—H10A	0.9700	C44—C45	1.353 (17)
C10—H10B	0.9700	C44—H44	0.9300
C11—H11A	0.9600	C45—C46	1.533 (16)
C11—H11B	0.9600	C46—H46A	0.9700
C11—H11C	0.9600	C46—H46B	0.9700
C12—C13	1.513 (15)	C47—C48	1.546 (18)
C12—H12A	0.9700	C47—H47A	0.9700
C12—H12B	0.9700	C47—H47B	0.9700

C13—H13A	0.9600	C48—H48A	0.9600
C13—H13B	0.9600	C48—H48B	0.9600
C13—H13C	0.9600	C48—H48C	0.9600
N2—C21	1.521 (13)	C49—C50	1.506 (15)
N2—C25	1.522 (13)	C49—H49A	0.9700
N2—C23	1.523 (14)	C49—H49B	0.9700
N2—C20	1.531 (13)	C50—H50A	0.9600
C14—C19	1.385 (16)	C50—H50B	0.9600
C14—C15	1.394 (17)	C50—H50C	0.9600
C14—H14	0.9300	C51—C52	1.540 (17)
C15—C16	1.393 (18)	C51—H51A	0.9700
C15—H15	0.9300	C51—H51B	0.9700
C16—C17	1.381 (17)	C52—H52A	0.9600
C16—H16	0.9300	C52—H52B	0.9600
C17—C18	1.382 (17)	C52—H52C	0.9600
O7—Mo1—O1	104.2 (4)	H11B—C11—H11C	109.5
O7—Mo1—O12	100.9 (3)	N1—C12—C13	116.6 (9)
O1—Mo1—O12	102.8 (3)	N1—C12—H12A	108.1
O7—Mo1—O2	101.4 (3)	C13—C12—H12A	108.1
O1—Mo1—O2	97.1 (3)	N1—C12—H12B	108.1
O12—Mo1—O2	145.3 (3)	C13—C12—H12B	108.1
O7—Mo1—O8	158.2 (3)	H12A—C12—H12B	107.3
O1—Mo1—O8	97.4 (3)	C12—C13—H13A	109.5
O12—Mo1—O8	76.5 (3)	C12—C13—H13B	109.5
O2—Mo1—O8	72.9 (2)	H13A—C13—H13B	109.5
O7—Mo1—O11	86.4 (3)	C12—C13—H13C	109.5
O1—Mo1—O11	165.8 (3)	H13A—C13—H13C	109.5
O12—Mo1—O11	84.0 (3)	H13B—C13—H13C	109.5
O2—Mo1—O11	71.2 (2)	C21—N2—C25	105.9 (9)
O8—Mo1—O11	71.8 (2)	C21—N2—C23	110.7 (9)
O6—Mo2—O13	103.2 (3)	C25—N2—C23	110.4 (9)
O6—Mo2—O11^{i}	102.5 (3)	C21—N2—C20	113.0 (9)
O13—Mo2—O11^{i}	96.5 (3)	C25—N2—C20	110.5 (9)
O6—Mo2—O2	100.7 (3)	C23—N2—C20	106.5 (9)
O13—Mo2—O2	97.1 (3)	C19—C14—C15	122.1 (12)
O11^{i}—Mo2—O2	149.6 (3)	C19—C14—H14	119.0
O6—Mo2—O8	100.2 (3)	C15—C14—H14	119.0
O13—Mo2—O8	156.6 (3)	C16—C15—C14	119.5 (13)
O11^{i}—Mo2—O8	78.5 (3)	C16—C15—H15	120.3
O2—Mo2—O8	78.3 (3)	C14—C15—H15	120.3
O6—Mo2—O8^{i}	175.8 (3)	C17—C16—C15	119.3 (13)
O13—Mo2—O8^{i}	80.6 (3)	C17—C16—H16	120.3
O11^{i}—Mo2—O8^{i}	78.6 (3)	C15—C16—H16	120.3
O2—Mo2—O8^{i}	76.9 (3)	C16—C17—C18	120.7 (13)
O8—Mo2—O8^{i}	75.9 (3)	C16—C17—H17	119.7
O4—Mo3—O9	104.8 (3)	C18—C17—H17	119.7
O4—Mo3—O3	100.4 (3)	C17—C18—C19	121.2 (13)

O9—Mo3—O3	100.3 (3)	C17—C18—H18	119.4
O4—Mo3—O11	101.1 (3)	C19—C18—H18	119.4
O9—Mo3—O11	98.8 (3)	C14—C19—C18	117.1 (12)
O3—Mo3—O11	146.4 (3)	C14—C19—C20	122.1 (12)
O4—Mo3—O8^{i}	159.9 (3)	C18—C19—C20	120.8 (12)
O9—Mo3—O8^{i}	95.2 (3)	C19—C20—N2	115.3 (10)
O3—Mo3—O8^{i}	77.6 (3)	C19—C20—H20A	108.4
O11—Mo3—O8^{i}	73.4 (2)	N2—C20—H20A	108.4
O4—Mo3—O2	88.1 (3)	C19—C20—H20B	108.4
O9—Mo3—O2	165.8 (3)	N2—C20—H20B	108.4
O3—Mo3—O2	82.9 (3)	H20A—C20—H20B	107.5
O11—Mo3—O2	72.4 (2)	N2—C21—C22	114.9 (10)
O8^{i}—Mo3—O2	71.8 (2)	N2—C21—H21A	108.5
O5—Mo4—O10	105.4 (4)	C22—C21—H21A	108.5
O5—Mo4—O12^{i}	98.7 (3)	N2—C21—H21B	108.5
O10—Mo4—O12^{i}	103.1 (3)	C22—C21—H21B	108.5
O5—Mo4—O3	97.8 (3)	H21A—C21—H21B	107.5
O10—Mo4—O3	102.0 (3)	C21—C22—H22A	109.5
O12^{i}—Mo4—O3	144.9 (3)	C21—C22—H22B	109.5
O5—Mo4—O13	163.6 (3)	H22A—C22—H22B	109.5
O10—Mo4—O13	91.0 (3)	C21—C22—H22C	109.5
O12^{i}—Mo4—O13	78.1 (3)	H22A—C22—H22C	109.5
O3—Mo4—O13	77.3 (3)	H22B—C22—H22C	109.5
O5—Mo4—O8^{i}	93.1 (3)	C24—C23—N2	116.4 (10)
O10—Mo4—O8^{i}	161.4 (3)	C24—C23—H23A	108.2
O12^{i}—Mo4—O8^{i}	73.8 (2)	N2—C23—H23A	108.2
O3—Mo4—O8^{i}	74.6 (3)	C24—C23—H23B	108.2
O13—Mo4—O8^{i}	70.5 (2)	N2—C23—H23B	108.2
O15—Mo5—O21	103.8 (4)	H23A—C23—H23B	107.4
O15—Mo5—O24	102.9 (3)	C23—C24—H24A	109.5
O21—Mo5—O24	94.6 (3)	C23—C24—H24B	109.5
O15—Mo5—O14	101.1 (3)	H24A—C24—H24B	109.5
O21—Mo5—O14	95.9 (3)	C23—C24—H24C	109.5
O24—Mo5—O14	150.7 (3)	H24A—C24—H24C	109.5
O15—Mo5—O25	101.1 (3)	H24B—C24—H24C	109.5
O21—Mo5—O25	155.1 (3)	C26—C25—N2	116.1 (10)
O24—Mo5—O25	80.2 (3)	C26—C25—H25A	108.3
O14—Mo5—O25	78.8 (3)	N2—C25—H25A	108.3
O15—Mo5—O25^{ii}	177.6 (3)	C26—C25—H25B	108.3
O21—Mo5—O25^{ii}	78.4 (3)	N2—C25—H25B	108.3
O24—Mo5—O25^{ii}	77.8 (3)	H25A—C25—H25B	107.4
O14—Mo5—O25^{ii}	77.6 (3)	C25—C26—H26A	109.5
O25—Mo5—O25^{ii}	76.7 (3)	C25—C26—H26B	109.5
O19—Mo6—O17	103.1 (4)	H26A—C26—H26B	109.5
O19—Mo6—O22	101.3 (4)	C25—C26—H26C	109.5

O17—Mo6—O22	101.0 (4)	H26A—C26—H26C	109.5
O19—Mo6—O14	101.8 (4)	H26B—C26—H26C	109.5
O17—Mo6—O14	96.3 (3)	C33—N3—C36	104.7 (8)
O22—Mo6—O14	147.1 (3)	C33—N3—C38	111.9 (8)
O19—Mo6—O25	160.3 (4)	C36—N3—C38	111.3 (9)
O17—Mo6—O25	96.3 (3)	C33—N3—C34	110.3 (9)
O22—Mo6—O25	77.4 (3)	C36—N3—C34	111.9 (9)
O14—Mo6—O25	73.0 (3)	C38—N3—C34	106.8 (9)
O19—Mo6—O24^{ii}	88.1 (3)	C32—C27—C28	121.8 (12)
O17—Mo6—O24^{ii}	165.1 (3)	C32—C27—H27	119.1
O22—Mo6—O24^{ii}	86.2 (3)	C28—C27—H27	119.1
O14—Mo6—O24^{ii}	71.5 (3)	C29—C28—C27	117.4 (12)
O25—Mo6—O24^{ii}	72.3 (3)	C29—C28—H28	121.3
O20—Mo7—O23	104.5 (4)	C27—C28—H28	121.3
O20—Mo7—O22^{ii}	101.6 (4)	C30—C29—C28	121.5 (13)
O23—Mo7—O22^{ii}	98.2 (4)	C30—C29—H29	119.2
O20—Mo7—O18	103.7 (3)	C28—C29—H29	119.2
O23—Mo7—O18	97.6 (4)	C29—C30—C31	120.5 (12)
O22^{ii}—Mo7—O18	145.7 (3)	C29—C30—H30	119.7
O20—Mo7—O21	90.9 (4)	C31—C30—H30	119.7
O23—Mo7—O21	164.6 (4)	C30—C31—C32	120.4 (12)
O22^{ii}—Mo7—O21	79.0 (3)	C30—C31—H31	119.8
O18—Mo7—O21	77.8 (3)	C32—C31—H31	119.8
O20—Mo7—O25^{ii}	160.5 (4)	C27—C32—C31	118.4 (11)
O23—Mo7—O25^{ii}	95.0 (4)	C27—C32—C33	117.4 (11)
O22^{ii}—Mo7—O25^{ii}	74.3 (3)	C31—C32—C33	124.0 (11)
O18—Mo7—O25^{ii}	74.1 (3)	N3—C33—C32	118.4 (9)
O21—Mo7—O25^{ii}	69.6 (3)	N3—C33—H33A	107.7
O16—Mo8—O26	104.4 (4)	C32—C33—H33A	107.7
O16—Mo8—O18	103.0 (4)	N3—C33—H33B	107.7
O26—Mo8—O18	101.7 (4)	C32—C33—H33B	107.7
O16—Mo8—O24^{ii}	97.2 (4)	H33A—C33—H33B	107.1
O26—Mo8—O24^{ii}	101.0 (3)	C35—C34—N3	114.5 (10)
O18—Mo8—O24^{ii}	144.7 (3)	C35—C34—H34A	108.6
O16—Mo8—O14	164.7 (3)	N3—C34—H34A	108.6
O26—Mo8—O14	88.0 (3)	C35—C34—H34B	108.6
O18—Mo8—O14	82.9 (3)	N3—C34—H34B	108.6
O24^{ii}—Mo8—O14	71.2 (3)	H34A—C34—H34B	107.6
O16—Mo8—O25^{ii}	95.8 (3)	C34—C35—H35A	109.5
O26—Mo8—O25^{ii}	159.6 (3)	C34—C35—H35B	109.5
O18—Mo8—O25^{ii}	76.7 (3)	H35A—C35—H35B	109.5
O24^{ii}—Mo8—O25^{ii}	72.6 (3)	C34—C35—H35C	109.5
O14—Mo8—O25^{ii}	71.6 (3)	H35A—C35—H35C	109.5
Mo2—O2—Mo1	110.0 (3)	H35B—C35—H35C	109.5

Mo2—O2—Mo3	111.2 (3)	N3—C36—C37	115.0 (9)
Mo1—O2—Mo3	104.4 (3)	N3—C36—H36A	108.5
Mo3—O3—Mo4	115.9 (4)	C37—C36—H36A	108.5
Mo2—O8—Mo3^{i}	92.1 (2)	N3—C36—H36B	108.5
Mo2—O8—Mo1	91.6 (2)	C37—C36—H36B	108.5
Mo3^{i}—O8—Mo1	164.2 (3)	H36A—C36—H36B	107.5
Mo2—O8—Mo2^{i}	104.1 (3)	C36—C37—H37A	109.5
Mo3^{i}—O8—Mo2^{i}	97.1 (3)	C36—C37—H37B	109.5
Mo1—O8—Mo2^{i}	96.9 (2)	H37A—C37—H37B	109.5
Mo2—O8—Mo4^{i}	164.5 (3)	C36—C37—H37C	109.5
Mo3^{i}—O8—Mo4^{i}	86.0 (2)	H37A—C37—H37C	109.5
Mo1—O8—Mo4^{i}	86.3 (2)	H37B—C37—H37C	109.5
Mo2^{i}—O8—Mo4^{i}	91.4 (2)	C39—C38—N3	115.7 (10)
Mo2^{i}—O11—Mo3	110.1 (3)	C39—C38—H38A	108.4
Mo2^{i}—O11—Mo1	110.0 (3)	N3—C38—H38A	108.4
Mo3—O11—Mo1	102.4 (3)	C39—C38—H38B	108.4
Mo1—O12—Mo4^{i}	118.7 (3)	N3—C38—H38B	108.4
Mo2—O13—Mo4	117.5 (3)	H38A—C38—H38B	107.4
Mo5—O14—Mo6	108.7 (3)	C38—C39—H39A	109.5
Mo5—O14—Mo8	111.6 (3)	C38—C39—H39B	109.5
Mo6—O14—Mo8	104.0 (3)	H39A—C39—H39B	109.5
Mo8—O18—Mo7	118.2 (4)	C38—C39—H39C	109.5
Mo5—O21—Mo7	119.8 (4)	H39A—C39—H39C	109.5
Mo6—O22—Mo7^{ii}	118.5 (4)	H39B—C39—H39C	109.5
Mo5—O24—Mo8^{ii}	108.9 (3)	C51—N4—C47	105.0 (9)
Mo5—O24—Mo6^{ii}	110.9 (3)	C51—N4—C46	111.6 (9)
Mo8^{ii}—O24—Mo6^{ii}	103.5 (3)	C47—N4—C46	111.5 (10)
Mo5—O25—Mo6	92.8 (3)	C51—N4—C49	111.2 (10)
Mo5—O25—Mo8^{ii}	91.7 (3)	C47—N4—C49	110.6 (10)
Mo6—O25—Mo8^{ii}	164.5 (4)	C46—N4—C49	107.0 (9)
Mo5—O25—Mo5^{ii}	103.3 (3)	C41—C40—C45	120.7 (14)
Mo6—O25—Mo5^{ii}	96.6 (3)	C41—C40—H40	119.7
Mo8^{ii}—O25—Mo5^{ii}	96.7 (3)	C45—C40—H40	119.7
Mo5—O25—Mo7^{ii}	164.5 (4)	C42—C41—C40	120.8 (14)
Mo6—O25—Mo7^{ii}	86.4 (2)	C42—C41—H41	119.6
Mo8^{ii}—O25—Mo7^{ii}	85.3 (2)	C40—C41—H41	119.6
Mo5^{ii}—O25—Mo7^{ii}	92.2 (3)	C41—C42—C43	118.7 (14)
C12—N1—C10	112.1 (9)	C41—C42—H42	120.6
C12—N1—C8	106.9 (9)	C43—C42—H42	120.6
C10—N1—C8	108.9 (9)	C42—C43—C44	120.7 (15)
C12—N1—C7	108.6 (8)	C42—C43—H43	119.6
C10—N1—C7	109.2 (8)	C44—C43—H43	119.6
C8—N1—C7	111.1 (8)	C45—C44—C43	120.9 (13)
C2—C1—C6	122.0 (11)	C45—C44—H44	119.5

C2—C1—H1	119.0	C43—C44—H44	119.5
C6—C1—H1	119.0	C44—C45—C40	118.0 (13)
C1—C2—C3	120.4 (11)	C44—C45—C46	122.0 (13)
C1—C2—H2	119.8	C40—C45—C46	119.9 (13)
C3—C2—H2	119.8	N4—C46—C45	118.4 (10)
C4—C3—C2	118.6 (11)	N4—C46—H46A	107.7
C4—C3—H3	120.7	C45—C46—H46A	107.7
C2—C3—H3	120.7	N4—C46—H46B	107.7
C3—C4—C5	120.7 (11)	C45—C46—H46B	107.7
C3—C4—H4	119.6	H46A—C46—H46B	107.1
C5—C4—H4	119.6	N4—C47—C48	113.6 (11)
C6—C5—C4	120.7 (11)	N4—C47—H47A	108.8
C6—C5—H5	119.7	C48—C47—H47A	108.8
C4—C5—H5	119.7	N4—C47—H47B	108.8
C5—C6—C1	117.6 (11)	C48—C47—H47B	108.8
C5—C6—C7	122.2 (10)	H47A—C47—H47B	107.7
C1—C6—C7	120.0 (10)	C47—C48—H48A	109.5
C6—C7—N1	115.4 (9)	C47—C48—H48B	109.5
C6—C7—H7A	108.4	H48A—C48—H48B	109.5
N1—C7—H7A	108.4	C47—C48—H48C	109.5
C6—C7—H7B	108.4	H48A—C48—H48C	109.5
N1—C7—H7B	108.4	H48B—C48—H48C	109.5
H7A—C7—H7B	107.5	C50—C49—N4	114.6 (10)
N1—C8—C9	113.6 (10)	C50—C49—H49A	108.6
N1—C8—H8A	108.9	N4—C49—H49A	108.6
C9—C8—H8A	108.9	C50—C49—H49B	108.6
N1—C8—H8B	108.9	N4—C49—H49B	108.6
C9—C8—H8B	108.9	H49A—C49—H49B	107.6
H8A—C8—H8B	107.7	C49—C50—H50A	109.5
C8—C9—H9A	109.5	C49—C50—H50B	109.5
C8—C9—H9B	109.5	H50A—C50—H50B	109.5
H9A—C9—H9B	109.5	C49—C50—H50C	109.5
C8—C9—H9C	109.5	H50A—C50—H50C	109.5
H9A—C9—H9C	109.5	H50B—C50—H50C	109.5
H9B—C9—H9C	109.5	N4—C51—C52	116.2 (11)
N1—C10—C11	113.8 (9)	N4—C51—H51A	108.2
N1—C10—H10A	108.8	C52—C51—H51A	108.2
C11—C10—H10A	108.8	N4—C51—H51B	108.2
N1—C10—H10B	108.8	C52—C51—H51B	108.2
C11—C10—H10B	108.8	H51A—C51—H51B	107.4
H10A—C10—H10B	107.7	C51—C52—H52A	109.5
C10—C11—H11A	109.5	C51—C52—H52B	109.5
C10—C11—H11B	109.5	H52A—C52—H52B	109.5
H11A—C11—H11B	109.5	C51—C52—H52C	109.5
C10—C11—H11C	109.5	H52A—C52—H52C	109.5
H11A—C11—H11C	109.5	H52B—C52—H52C	109.5
O6—Mo2—O2—Mo1	75.1 (4)	O25^{ii}—Mo7—O18—Mo8	−21.7 (4)
O13—Mo2—O2—Mo1	−180.0 (3)	O15—Mo5—O21—Mo7	−177.6 (4)

O11^{i}—Mo2—O2—Mo1	−64.1 (6)	O24—Mo5—O21—Mo7	77.9 (4)
O8—Mo2—O2—Mo1	−23.3 (3)	O14—Mo5—O21—Mo7	−74.6 (4)
O8^{i}—Mo2—O2—Mo1	−101.4 (3)	O25—Mo5—O21—Mo7	1.4 (9)
O6—Mo2—O2—Mo3	−169.8 (3)	O25^{ii}—Mo5—O21—Mo7	1.4 (3)
O13—Mo2—O2—Mo3	−64.8 (3)	O20—Mo7—O21—Mo5	179.8 (4)
O11^{i}—Mo2—O2—Mo3	51.0 (6)	O23—Mo7—O21—Mo5	2.1 (15)
O8—Mo2—O2—Mo3	91.9 (3)	O22^{ii}—Mo7—O21—Mo5	−78.6 (4)
O8^{i}—Mo2—O2—Mo3	13.8 (3)	O18—Mo7—O21—Mo5	76.0 (4)
O7—Mo1—O2—Mo2	179.9 (4)	O25^{ii}—Mo7—O21—Mo5	−1.4 (3)
O1—Mo1—O2—Mo2	−73.9 (4)	O19—Mo6—O22—Mo7^{ii}	177.1 (5)
O12—Mo1—O2—Mo2	51.0 (6)	O17—Mo6—O22—Mo7^{ii}	−76.9 (5)
O8—Mo1—O2—Mo2	21.6 (3)	O14—Mo6—O22—Mo7^{ii}	43.4 (9)
O11—Mo1—O2—Mo2	97.7 (3)	O25—Mo6—O22—Mo7^{ii}	17.2 (4)
O7—Mo1—O2—Mo3	60.5 (4)	O24^{ii}—Mo6—O22—Mo7^{ii}	89.9 (4)
O1—Mo1—O2—Mo3	166.6 (3)	O15—Mo5—O24—Mo8^{ii}	77.0 (4)
O12—Mo1—O2—Mo3	−68.4 (6)	O21—Mo5—O24—Mo8^{ii}	−177.8 (4)
O8—Mo1—O2—Mo3	−97.8 (3)	O14—Mo5—O24—Mo8^{ii}	−67.2 (7)
O11—Mo1—O2—Mo3	−21.7 (2)	O25—Mo5—O24—Mo8^{ii}	−22.3 (3)
O4—Mo3—O2—Mo2	165.4 (4)	O25^{ii}—Mo5—O24—Mo8^{ii}	−100.7 (4)
O9—Mo3—O2—Mo2	−39.2 (13)	O15—Mo5—O24—Mo6^{ii}	−169.8 (3)
O3—Mo3—O2—Mo2	64.6 (3)	O21—Mo5—O24—Mo6^{ii}	−64.5 (4)
O11—Mo3—O2—Mo2	−92.3 (3)	O14—Mo5—O24—Mo6^{ii}	46.0 (8)
O8^{i}—Mo3—O2—Mo2	−14.6 (3)	O25—Mo5—O24—Mo6^{ii}	90.9 (4)
O4—Mo3—O2—Mo1	−76.0 (3)	O25^{ii}—Mo5—O24—Mo6^{ii}	12.6 (3)
O9—Mo3—O2—Mo1	79.4 (12)	O15—Mo5—O25—Mo6	81.5 (3)
O3—Mo3—O2—Mo1	−176.8 (3)	O21—Mo5—O25—Mo6	−97.5 (7)
O11—Mo3—O2—Mo1	26.2 (3)	O24—Mo5—O25—Mo6	−177.2 (3)
O8^{i}—Mo3—O2—Mo1	104.0 (3)	O14—Mo5—O25—Mo6	−17.8 (3)
O4—Mo3—O3—Mo4	178.3 (4)	O25^{ii}—Mo5—O25—Mo6	−97.5 (3)
O9—Mo3—O3—Mo4	71.0 (4)	O15—Mo5—O25—Mo8^{ii}	−83.7 (3)
O11—Mo3—O3—Mo4	−52.7 (7)	O21—Mo5—O25—Mo8^{ii}	97.3 (7)
O8^{i}—Mo3—O3—Mo4	−22.1 (3)	O24—Mo5—O25—Mo8^{ii}	17.6 (3)
O2—Mo3—O3—Mo4	−95.0 (4)	O14—Mo5—O25—Mo8^{ii}	177.0 (3)
O5—Mo4—O3—Mo3	−69.7 (4)	O25^{ii}—Mo5—O25—Mo8^{ii}	97.3 (3)
O10—Mo4—O3—Mo3	−177.4 (4)	O15—Mo5—O25—Mo5^{ii}	179.0 (3)
O12^{i}—Mo4—O3—Mo3	47.8 (7)	O21—Mo5—O25—Mo5^{ii}	0.0 (8)
O13—Mo4—O3—Mo3	94.3 (4)	O24—Mo5—O25—Mo5^{ii}	−79.7 (3)
O8^{i}—Mo4—O3—Mo3	21.4 (3)	O14—Mo5—O25—Mo5^{ii}	79.7 (3)
O6—Mo2—O8—Mo3^{i}	84.0 (3)	O25^{ii}—Mo5—O25—Mo5^{ii}	0.0
O13—Mo2—O8—Mo3^{i}	−96.3 (7)	O15—Mo5—O25—Mo7^{ii}	−5.2 (14)
O11^{i}—Mo2—O8—Mo3^{i}	−16.8 (2)	O21—Mo5—O25—Mo7^{ii}	175.8 (11)

O2—Mo2—O8—Mo3^{i}	−177.1 (3)	O24—Mo5—O25—Mo7^{ii}	96.2 (14)
O8^{i}—Mo2—O8—Mo3^{i}	−97.8 (3)	O14—Mo5—O25—Mo7^{ii}	−104.5 (14)
O6—Mo2—O8—Mo1	−80.7 (3)	O25^{ii}—Mo5—O25—Mo7^{ii}	175.8 (16)
O13—Mo2—O8—Mo1	99.0 (7)	O19—Mo6—O25—Mo5	95.2 (10)
O11^{i}—Mo2—O8—Mo1	178.5 (3)	O17—Mo6—O25—Mo5	−76.5 (4)
O2—Mo2—O8—Mo1	18.2 (2)	O22—Mo6—O25—Mo5	−176.4 (4)
O8^{i}—Mo2—O8—Mo1	97.5 (3)	O14—Mo6—O25—Mo5	18.2 (3)
O6—Mo2—O8—Mo2^{i}	−178.2 (3)	O24^{ii}—Mo6—O25—Mo5	93.6 (3)
O13—Mo2—O8—Mo2^{i}	1.5 (8)	O19—Mo6—O25—Mo8^{ii}	−157.9 (12)
O11^{i}—Mo2—O8—Mo2^{i}	81.0 (3)	O17—Mo6—O25—Mo8^{ii}	30.4 (14)
O2—Mo2—O8—Mo2^{i}	−79.3 (3)	O22—Mo6—O25—Mo8^{ii}	−69.5 (13)
O8^{i}—Mo2—O8—Mo2^{i}	0.0	O14—Mo6—O25—Mo8^{ii}	125.0 (14)
O6—Mo2—O8—Mo4^{i}	1.4 (13)	O24^{ii}—Mo6—O25—Mo8^{ii}	−159.5 (14)
O13—Mo2—O8—Mo4^{i}	−179.0 (10)	O19—Mo6—O25—Mo5^{ii}	−8.5 (11)
O11^{i}—Mo2—O8—Mo4^{i}	−99.5 (13)	O17—Mo6—O25—Mo5^{ii}	179.8 (3)
O2—Mo2—O8—Mo4^{i}	100.2 (13)	O22—Mo6—O25—Mo5^{ii}	79.9 (3)
O8^{i}—Mo2—O8—Mo4^{i}	179.5 (15)	O14—Mo6—O25—Mo5^{ii}	−85.6 (3)
O7—Mo1—O8—Mo2	−96.1 (8)	O24^{ii}—Mo6—O25—Mo5^{ii}	−10.1 (2)
O1—Mo1—O8—Mo2	76.8 (3)	O19—Mo6—O25—Mo7^{ii}	−100.3 (10)
O12—Mo1—O8—Mo2	178.3 (3)	O17—Mo6—O25—Mo7^{ii}	88.0 (3)
O2—Mo1—O8—Mo2	−18.5 (2)	O22—Mo6—O25—Mo7^{ii}	−11.9 (3)
O11—Mo1—O8—Mo2	−93.8 (3)	O14—Mo6—O25—Mo7^{ii}	−177.3 (3)
O7—Mo1—O8—Mo3^{i}	160.3 (10)	O24^{ii}—Mo6—O25—Mo7^{ii}	−101.9 (3)
O1—Mo1—O8—Mo3^{i}	−26.8 (12)	C6—C1—C2—C3	−1.9 (19)
O12—Mo1—O8—Mo3^{i}	74.7 (12)	C1—C2—C3—C4	0.1 (18)
O2—Mo1—O8—Mo3^{i}	−122.0 (12)	C2—C3—C4—C5	1.0 (18)
O11—Mo1—O8—Mo3^{i}	162.7 (12)	C3—C4—C5—C6	−0.2 (18)
O7—Mo1—O8—Mo2^{i}	8.2 (9)	C4—C5—C6—C1	−1.5 (17)
O1—Mo1—O8—Mo2^{i}	−178.9 (3)	C4—C5—C6—C7	−176.5 (10)
O12—Mo1—O8—Mo2^{i}	−77.4 (3)	C2—C1—C6—C5	2.6 (18)
O2—Mo1—O8—Mo2^{i}	85.9 (3)	C2—C1—C6—C7	177.7 (11)
O11—Mo1—O8—Mo2^{i}	10.6 (2)	C5—C6—C7—N1	−92.9 (13)
O7—Mo1—O8—Mo4^{i}	99.2 (8)	C1—C6—C7—N1	92.3 (12)
O1—Mo1—O8—Mo4^{i}	−87.9 (3)	C12—N1—C7—C6	58.5 (12)
O12—Mo1—O8—Mo4^{i}	13.6 (2)	C10—N1—C7—C6	−179.0 (9)
O2—Mo1—O8—Mo4^{i}	176.9 (3)	C8—N1—C7—C6	−58.8 (12)
O11—Mo1—O8—Mo4^{i}	101.6 (2)	C12—N1—C8—C9	175.2 (9)
O4—Mo3—O11—Mo2^{i}	180.0 (3)	C10—N1—C8—C9	53.9 (13)
O9—Mo3—O11—Mo2^{i}	−72.9 (4)	C7—N1—C8—C9	−66.4 (12)
O3—Mo3—O11—Mo2^{i}	51.1 (6)	C12—N1—C10—C11	53.7 (13)
O8^{i}—Mo3—O11—Mo2^{i}	19.9 (3)	C8—N1—C10—C11	171.8 (10)

O2—Mo3—O11—Mo2^{i}	95.6 (3)	C7—N1—C10—C11	−66.7 (12)
O4—Mo3—O11—Mo1	63.0 (3)	C10—N1—C12—C13	51.4 (13)
O9—Mo3—O11—Mo1	170.1 (3)	C8—N1—C12—C13	−67.8 (12)
O3—Mo3—O11—Mo1	−65.9 (6)	C7—N1—C12—C13	172.2 (10)
O8^{i}—Mo3—O11—Mo1	−97.1 (3)	C19—C14—C15—C16	3(2)
O2—Mo3—O11—Mo1	−21.4 (2)	C14—C15—C16—C17	−2(2)
O7—Mo1—O11—Mo2^{i}	165.2 (4)	C15—C16—C17—C18	0(2)
O1—Mo1—O11—Mo2^{i}	−55.5 (13)	C16—C17—C18—C19	2(2)
O12—Mo1—O11—Mo2^{i}	63.9 (3)	C15—C14—C19—C18	−2.3 (19)
O2—Mo1—O11—Mo2^{i}	−91.5 (3)	C15—C14—C19—C20	178.9 (12)
O8—Mo1—O11—Mo2^{i}	−13.9 (3)	C17—C18—C19—C14	−0.1 (19)
O7—Mo1—O11—Mo3	−77.7 (3)	C17—C18—C19—C20	178.7 (12)
O1—Mo1—O11—Mo3	61.5 (13)	C14—C19—C20—N2	−93.2 (14)
O12—Mo1—O11—Mo3	−179.1 (3)	C18—C19—C20—N2	88.0 (15)
O2—Mo1—O11—Mo3	25.6 (3)	C21—N2—C20—C19	−64.2 (13)
O8—Mo1—O11—Mo3	103.1 (3)	C25—N2—C20—C19	54.3 (13)
O7—Mo1—O12—Mo4^{i}	−177.8 (4)	C23—N2—C20—C19	174.1 (10)
O1—Mo1—O12—Mo4^{i}	74.8 (5)	C25—N2—C21—C22	173.5 (10)
O2—Mo1—O12—Mo4^{i}	−48.8 (7)	C23—N2—C21—C22	53.9 (13)
O8—Mo1—O12—Mo4^{i}	−19.9 (3)	C20—N2—C21—C22	−65.4 (13)
O11—Mo1—O12—Mo4^{i}	−92.6 (4)	C21—N2—C23—C24	55.8 (13)
O6—Mo2—O13—Mo4	177.6 (4)	C25—N2—C23—C24	−61.1 (13)
O11^{i}—Mo2—O13—Mo4	−77.9 (4)	C20—N2—C23—C24	179.0 (10)
O2—Mo2—O13—Mo4	74.9 (4)	C21—N2—C25—C26	−170.7 (10)
O8—Mo2—O13—Mo4	−2.1 (10)	C23—N2—C25—C26	−50.9 (13)
O8^{i}—Mo2—O13—Mo4	−0.6 (3)	C20—N2—C25—C26	66.6 (13)
O5—Mo4—O13—Mo2	−3.0 (13)	C32—C27—C28—C29	−1.4 (18)
O10—Mo4—O13—Mo2	−179.4 (4)	C27—C28—C29—C30	0.2 (18)
O12^{i}—Mo4—O13—Mo2	77.4 (4)	C28—C29—C30—C31	0.9 (19)
O3—Mo4—O13—Mo2	−77.4 (4)	C29—C30—C31—C32	−0.8 (19)
O8^{i}—Mo4—O13—Mo2	0.6 (3)	C28—C27—C32—C31	1.4 (17)
O15—Mo5—O14—Mo6	−77.0 (4)	C28—C27—C32—C33	−173.6 (10)
O21—Mo5—O14—Mo6	177.7 (4)	C30—C31—C32—C27	−0.3 (18)
O24—Mo5—O14—Mo6	67.5 (7)	C30—C31—C32—C33	174.4 (11)
O25—Mo5—O14—Mo6	22.3 (3)	C36—N3—C33—C32	174.5 (10)
O25^{ii}—Mo5—O14—Mo6	101.0 (4)	C38—N3—C33—C32	−64.8 (13)
O15—Mo5—O14—Mo8	168.9 (4)	C34—N3—C33—C32	53.9 (13)
O21—Mo5—O14—Mo8	63.6 (4)	C27—C32—C33—N3	−110.6 (12)
O24—Mo5—O14—Mo8	−46.6 (8)	C31—C32—C33—N3	74.6 (15)
O25—Mo5—O14—Mo8	−91.8 (4)	C33—N3—C34—C35	63.8 (12)
O25^{ii}—Mo5—O14—Mo8	−13.1 (3)	C36—N3—C34—C35	−52.3 (13)
O19—Mo6—O14—Mo5	179.1 (4)	C38—N3—C34—C35	−174.4 (10)
O17—Mo6—O14—Mo5	74.2 (4)	C33—N3—C36—C37	−177.5 (10)
O22—Mo6—O14—Mo5	−47.3 (7)	C38—N3—C36—C37	61.4 (13)
O25—Mo6—O14—Mo5	−20.5 (3)	C34—N3—C36—C37	−58.0 (13)

O24^{ii}—Mo6—O14—Mo5	−97.0 (4)	C33—N3—C38—C39	−58.5 (13)
O19—Mo6—O14—Mo8	−61.9 (4)	C36—N3—C38—C39	58.3 (13)
O17—Mo6—O14—Mo8	−166.8 (3)	C34—N3—C38—C39	−179.2 (10)
O22—Mo6—O14—Mo8	71.7 (6)	C45—C40—C41—C42	−4(3)
O25—Mo6—O14—Mo8	98.5 (3)	C40—C41—C42—C43	5(2)
O24^{ii}—Mo6—O14—Mo8	22.0 (3)	C41—C42—C43—C44	−2(2)
O16—Mo8—O14—Mo5	49.2 (15)	C42—C43—C44—C45	−1(2)
O26—Mo8—O14—Mo5	−166.7 (4)	C43—C44—C45—C40	1(2)
O18—Mo8—O14—Mo5	−64.6 (4)	C43—C44—C45—C46	−174.6 (12)
O24^{ii}—Mo8—O14—Mo5	91.0 (4)	C41—C40—C45—C44	1(2)
O25^{ii}—Mo8—O14—Mo5	13.7 (3)	C41—C40—C45—C46	176.9 (13)
O16—Mo8—O14—Mo6	−67.8 (14)	C51—N4—C46—C45	−57.5 (15)
O26—Mo8—O14—Mo6	76.3 (4)	C47—N4—C46—C45	59.6 (15)
O18—Mo8—O14—Mo6	178.4 (4)	C49—N4—C46—C45	−179.3 (11)
O24^{ii}—Mo8—O14—Mo6	−26.0 (3)	C44—C45—C46—N4	−93.8 (15)
O25^{ii}—Mo8—O14—Mo6	−103.4 (3)	C40—C45—C46—N4	90.2 (15)
O16—Mo8—O18—Mo7	−71.0 (5)	C51—N4—C47—C48	−172.7 (11)
O26—Mo8—O18—Mo7	−178.9 (4)	C46—N4—C47—C48	66.3 (14)
O24^{ii}—Mo8—O18—Mo7	52.1 (8)	C49—N4—C47—C48	−52.7 (14)
O14—Mo8—O18—Mo7	94.6 (4)	C51—N4—C49—C50	58.8 (14)
O25^{ii}—Mo8—O18—Mo7	21.9 (4)	C47—N4—C49—C50	−57.5 (14)
O20—Mo7—O18—Mo8	178.4 (5)	C46—N4—C49—C50	−179.2 (11)
O23—Mo7—O18—Mo8	71.4 (5)	C47—N4—C51—C52	172.4 (11)
O22^{ii}—Mo7—O18—Mo8	−45.3 (8)	C46—N4—C51—C52	−66.7 (14)
O21—Mo7—O18—Mo8	−93.7 (4)	C49—N4—C51—C52	52.7 (14)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C49—H49A···O19^{iii}	0.97	2.59	3.371 (15)	138
C46—H46B···O21^{iv}	0.97	2.60	3.098 (13)	112
C38—H38B···O12^{v}	0.97	2.56	3.508 (14)	166
C37—H37A···O12^{v}	0.96	2.29	3.199 (13)	157
C36—H36B···O6	0.97	2.45	3.144 (13)	128
C36—H36B···O1	0.97	2.54	3.381 (14)	146
C33—H33A···O1	0.97	2.29	3.212 (12)	158
C29—H29···O5^{vi}	0.93	2.48	3.177 (15)	132
C26—H26A···O23^{vii}	0.96	2.55	3.219 (15)	127
C25—H25A···O2^{vii}	0.97	2.37	3.037 (12)	126
C24—H24C···O4^{vii}	0.96	2.56	3.464 (16)	158
C23—H23A···O17^{viii}	0.97	2.40	3.360 (14)	169
C22—H22C···O20	0.96	2.59	3.326 (16)	134
C21—H21A···O3^{vii}	0.97	2.57	3.499 (14)	160
C18—H18···O20	0.93	2.48	3.370 (15)	160

C12—H12A···O4^{vi}	0.97	2.44	3.182 (13)	133
C10—H10B···O7^{ix}	0.97	2.50	3.320 (15)	142
C9—H9B···O17^{x}	0.96	2.42	3.209 (14)	139
C8—H8A···O16^{ix}	0.97	2.42	3.339 (15)	158
C7—H7A···O7^{ix}	0.97	2.40	3.221 (13)	142
C5—H5···O3^{vi}	0.93	2.49	3.320 (13)	149

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

Fig. 1

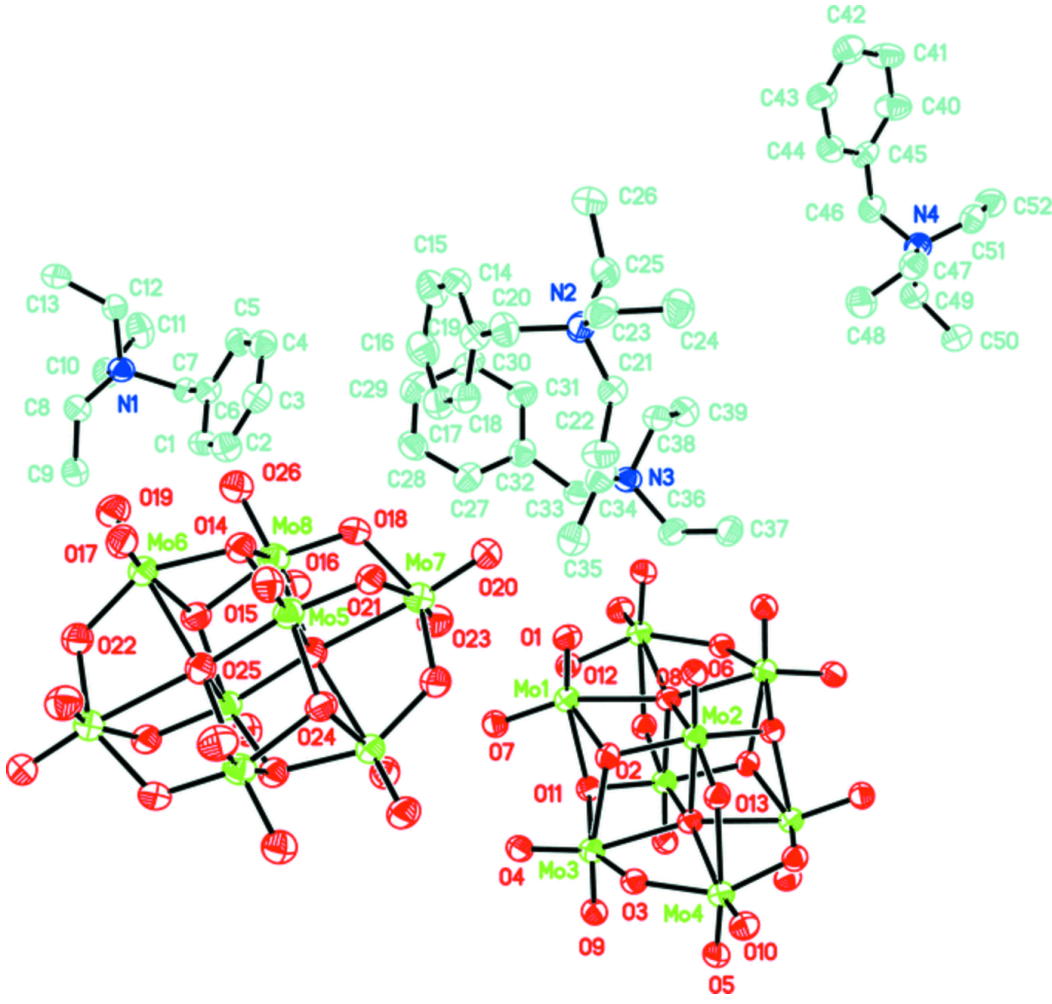
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Fig. 2