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Tetrakis(1-*n*-hexylpyridinium) octamolybdate

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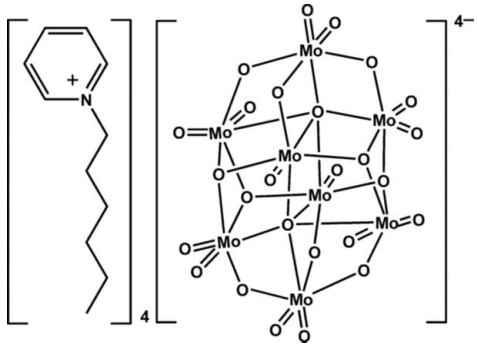
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.016 Å; R factor = 0.044; wR factor = 0.114; data-to-parameter ratio = 14.7.

The asymmetric unit of the title compound, $(C_{11}H_{18}N)_4[Mo_8O_{26}]$, contains two cations and one half-anion; the anion is centrosymmetric. The anion is a β-isomer. Although no classical hydrogen bonds are found, a large number of weak intermolecular C—H···O hydrogen bonds and van der Waals forces stabilize the packing of the ions.

Related literature

For related literature, see: Guo & Li (2007); Deng *et al.* (2005); Wang *et al.* (1993); Wilson *et al.* (1984).



Experimental

Crystal data

$(C_{11}H_{18}N)_4[Mo_8O_{26}]$
M_r = 1840.58
Monoclinic, $P2_1/n$
a = 15.474 (4) Å
b = 12.051 (3) Å
c = 16.592 (4) Å
β = 94.964 (5)°
V = 3082.4 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.65 mm^{-1}
T = 294 (2) K
0.22 × 0.20 × 0.16 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.698, T_{max} = 0.765
15694 measured reflections
5450 independent reflections
2782 reflections with $I > 2\sigma(I)$
R_{int} = 0.082

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.114
S = 0.95
5450 reflections
370 parameters
78 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C19—H19A···O4^{i}	0.97	2.60	3.391 (12)	139
C17—H17B···O6^{ii}	0.97	2.30	3.200 (11)	154
C17—H17A···O4	0.97	2.48	3.207 (11)	131
C17—H17A···O2	0.97	2.46	3.166 (10)	130
C16—H16···O5^{ii}	0.93	2.40	3.271 (11)	155
C15—H15···O9^{iii}	0.93	2.56	3.257 (13)	132
C12—H12···O2	0.93	2.40	3.243 (11)	151
C7—H7B···O3^{ii}	0.97	2.40	3.143 (12)	133
C5—H5···O1^{iv}	0.93	2.39	3.059 (13)	129
C4—H4···O8^{v}	0.93	2.56	3.295 (15)	136
C1—H1···O3^{ii}	0.93	2.50	3.295 (13)	144

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) $x, y, z+1$; (v) $x, y+1, z+1$.

Data collection: *SMART* (Bruker 1997); cell refinement: *SAINT* (Bruker 1997); data reduction: *SAINT*; 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: PK2017).

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supplementary materials

Acta Cryst. (2007). E**63**, m1471 [**doi:10.1107/S1600536807019423**]

Tetrakis(1-*n*-hexylpyridinium) octamolybdate

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

Comment

Polymolybdates have attracted considerable interest for application in selective catalysis of oxidation reactions with hydrogen peroxide. The synthesis and crystal structure reported here is part of this study (Guo and Li, 2007).

The title compound, (I), consists of a centrosymmetric β-octamolybdate anion and four n-hexylpyridinium cations. The structure of the anion is constructed from an array of eight edge-shared MoO_6 octahedra. The Mo–O bond lengths can be grouped into four sets: Mo–O(t) 1.672 (6)–1.694 (5) Å, Mo–O(μ2) 1.725 (5)–2.311 (5) Å, Mo–O(μ3) 1.939 (5)–2.311 (5) Å, Mo–O(μ5) 2.128 (5)–2.374 (5) Å. The molecule of the compound is shown in Fig. 1.

In the structure of (I), no classic hydrogen bonds are found, but there exist a number of weak C–H···O interactions (see Table 1). These are further loosely aggregated into a three-dimensional framework via van der Waals forces. A packing diagram for the structure of (I) is shown in Fig. 2.

Experimental

A solution of n-hexylpyridinium bromide (1.80 g, 7 mmol) in 10 ml of distilled water was added dropwise to a mixture of 20 ml aqueous solution of dihydrate sodium molybdate (1.2 g, 5 mmol) and 12% dilute hydrogen chloride (1.8 ml, 7 mmol) under stirring at 70°C. A white precipitate was immediately formed. After continuously stirring for 20 min, the resulting product was filtered, washed with water and dried at room temperature to produce the tetra-n-hexylpyridinium octamolybdate in 89% yield. Single crystals were separated from the above filtrate by slowly evaporating over a period of 1 d at 40°C.

Refinement

The H atoms bonded to C atoms were included in the refinement with a 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

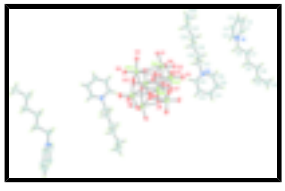


Fig. 1. A view of the structure of (I), showing the atom-numbering Scheme; displacement ellipsoids were drawn at the 30% probability level.

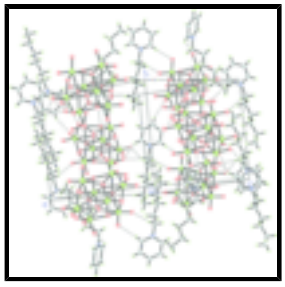


Fig. 2. Packing diagram showing hydrogen bonds interactions, viewed roughly down the diagonal between the a and c axes.

Tetrakis(1-n-hexylpyridinium) octamolybdate

Crystal data

$(C_{11}H_{18}N)_4[Mo_8O_{26}]$	F_{000} = 1816
M_r = 1840.58	D_x = 1.983 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2002 reflections
a = 15.474 (4) Å	θ = 2.4–21.6º
b = 12.051 (3) Å	μ = 1.65 mm^{-1}
c = 16.592 (4) Å	T = 294 (2) K
β = 94.964 (5)º	Block, colorless
V = 3082.4 (13) Å^3	0.22 × 0.20 × 0.16 mm
Z = 2	

Data collection

Bruker SMART CCD area-detector diffractometer	5450 independent reflections
Radiation source: fine-focus sealed tube	2782 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.082
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −18→11
T_{min} = 0.698, T_{max} = 0.765	k = −14→14
15694 measured reflections	l = −19→19

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.044	$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.114	$(\Delta/\sigma)_{max} < 0.001$
S = 0.95	$\Delta\rho_{max}$ = 0.63 e Å^{-3}

5450 reflections
370 parameters
78 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

$\Delta\rho_{min} = -0.62$ e Å^{-3}
Extinction correction: none

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	0.41536 (5)	0.20179 (6)	0.04058 (5)	0.0450 (2)
Mo2	0.48353 (5)	0.07732 (7)	0.20537 (5)	0.0499 (3)
Mo3	0.53068 (5)	0.16326 (7)	−0.12012 (5)	0.0476 (2)
Mo4	0.39661 (5)	−0.03796 (6)	−0.04320 (5)	0.0408 (2)
O1	0.4177 (4)	0.3339 (5)	0.0102 (4)	0.0603 (18)
O2	0.3120 (4)	0.1786 (5)	0.0627 (4)	0.0545 (17)
O3	0.5349 (4)	0.1230 (6)	0.2923 (4)	0.0670 (19)
O4	0.3787 (4)	0.0657 (5)	0.2242 (4)	0.0588 (18)
O5	0.4897 (4)	0.2894 (5)	−0.1449 (4)	0.0638 (19)
O6	0.6361 (4)	0.1711 (5)	−0.1393 (4)	0.0618 (19)
O7	0.2955 (3)	−0.0510 (5)	−0.0137 (3)	0.0504 (16)
O8	0.4487 (3)	−0.1747 (4)	0.0012 (3)	0.0404 (14)
O9	0.4740 (3)	0.2126 (5)	0.1435 (3)	0.0497 (16)
O10	0.4588 (3)	0.0179 (4)	0.0689 (3)	0.0412 (14)
O11	0.4034 (3)	0.1201 (4)	−0.0639 (3)	0.0424 (15)
O12	0.4840 (3)	0.0770 (5)	−0.2070 (3)	0.0494 (16)
O13	0.3885 (3)	−0.0793 (5)	−0.1431 (3)	0.0484 (15)
N1	0.2719 (6)	0.4703 (7)	0.8434 (5)	0.063 (2)
N2	0.1678 (5)	0.0741 (6)	0.2113 (5)	0.0553 (18)
C1	0.2063 (8)	0.5384 (10)	0.8243 (7)	0.078 (3)
H1	0.1574	0.5123	0.7935	0.094*
C2	0.2091 (9)	0.6445 (10)	0.8486 (9)	0.095 (4)
H2	0.1626	0.6918	0.8354	0.114*
C3	0.2804 (12)	0.6813 (11)	0.8924 (9)	0.113 (5)
H3	0.2836	0.7549	0.9092	0.136*
C4	0.3472 (10)	0.6120 (14)	0.9121 (9)	0.109 (5)
H4	0.3958	0.6377	0.9435	0.131*

C5	0.3441 (8)	0.5047 (11)	0.8863 (7)	0.081 (3)
H5	0.3906	0.4569	0.8981	0.097*
C6	0.2610 (6)	0.3530 (8)	0.8199 (6)	0.072 (2)
H6A	0.3178	0.3195	0.8179	0.086*
H6B	0.2312	0.3490	0.7661	0.086*
C7	0.2105 (6)	0.2877 (8)	0.8775 (6)	0.070 (2)
H7A	0.2436	0.2828	0.9297	0.084*
H7B	0.1564	0.3254	0.8848	0.084*
C8	0.1920 (6)	0.1735 (8)	0.8450 (7)	0.073 (2)
H8A	0.2466	0.1354	0.8405	0.088*
H8B	0.1628	0.1796	0.7911	0.088*
C9	0.1370 (7)	0.1045 (9)	0.8962 (7)	0.078 (2)
H9A	0.0820	0.1418	0.9006	0.094*
H9B	0.1659	0.0978	0.9502	0.094*
C10	0.1201 (7)	−0.0099 (9)	0.8613 (7)	0.084 (2)
H10A	0.0911	−0.0031	0.8073	0.101*
H10B	0.1751	−0.0471	0.8568	0.101*
C11	0.0653 (8)	−0.0788 (10)	0.9123 (7)	0.103 (4)
H11A	0.0974	−0.0949	0.9632	0.155*
H11B	0.0500	−0.1470	0.8848	0.155*
H11C	0.0136	−0.0387	0.9218	0.155*
C12	0.1944 (6)	0.0055 (8)	0.1554 (6)	0.053 (3)
H12	0.2310	0.0314	0.1180	0.064*
C13	0.1683 (6)	−0.1019 (9)	0.1532 (7)	0.067 (3)
H13	0.1884	−0.1507	0.1155	0.080*
C14	0.1128 (7)	−0.1372 (9)	0.2062 (8)	0.078 (3)
H14	0.0915	−0.2094	0.2032	0.094*
C15	0.0881 (7)	−0.0664 (11)	0.2643 (7)	0.091 (4)
H15	0.0536	−0.0917	0.3036	0.109*
C16	0.1140 (7)	0.0401 (10)	0.2642 (6)	0.076 (3)
H16	0.0942	0.0900	0.3012	0.092*
C17	0.1953 (6)	0.1912 (7)	0.2100 (6)	0.0611 (19)
H17A	0.2547	0.1946	0.1958	0.073*
H17B	0.1939	0.2221	0.2639	0.073*
C18	0.1401 (6)	0.2599 (8)	0.1522 (6)	0.068 (2)
H18A	0.0831	0.2671	0.1718	0.082*
H18B	0.1332	0.2220	0.1005	0.082*
C19	0.1760 (7)	0.3735 (9)	0.1398 (6)	0.074 (2)
H19A	0.1864	0.4092	0.1922	0.088*
H19B	0.2316	0.3658	0.1175	0.088*
C20	0.1206 (7)	0.4467 (9)	0.0863 (7)	0.084 (2)
H20A	0.0653	0.4567	0.1087	0.101*
H20B	0.1096	0.4118	0.0337	0.101*
C21	0.1629 (8)	0.5616 (9)	0.0757 (7)	0.092 (3)
H21A	0.1800	0.5928	0.1285	0.111*
H21B	0.2147	0.5526	0.0473	0.111*
C22	0.1029 (8)	0.6387 (11)	0.0300 (8)	0.119 (4)
H22A	0.0886	0.6101	−0.0235	0.179*
H22B	0.1302	0.7099	0.0265	0.179*

H22C	0.0510	0.6464	0.0572	0.179*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.0468 (5)	0.0387 (5)	0.0525 (6)	0.0037 (4)	0.0212 (4)	−0.0021 (4)
Mo2	0.0500 (5)	0.0571 (6)	0.0447 (6)	0.0045 (4)	0.0156 (4)	−0.0054 (4)
Mo3	0.0508 (5)	0.0426 (5)	0.0529 (6)	−0.0015 (4)	0.0245 (4)	0.0059 (4)
Mo4	0.0381 (4)	0.0379 (5)	0.0484 (5)	−0.0023 (4)	0.0154 (4)	−0.0029 (4)
O1	0.071 (4)	0.036 (4)	0.078 (5)	0.005 (3)	0.029 (4)	0.001 (3)
O2	0.048 (4)	0.059 (4)	0.061 (4)	0.003 (3)	0.027 (3)	0.004 (3)
O3	0.070 (5)	0.079 (5)	0.054 (4)	0.010 (4)	0.013 (3)	−0.016 (4)
O4	0.045 (4)	0.073 (5)	0.061 (4)	0.007 (3)	0.023 (3)	0.003 (4)
O5	0.073 (5)	0.053 (4)	0.069 (5)	0.004 (4)	0.027 (4)	0.017 (4)
O6	0.051 (4)	0.069 (5)	0.070 (5)	−0.008 (3)	0.031 (3)	0.013 (4)
O7	0.040 (4)	0.045 (4)	0.069 (4)	−0.004 (3)	0.021 (3)	−0.001 (3)
O8	0.043 (3)	0.038 (3)	0.043 (4)	0.001 (3)	0.020 (3)	−0.001 (3)
O9	0.050 (4)	0.045 (4)	0.056 (4)	−0.001 (3)	0.015 (3)	−0.013 (3)
O10	0.043 (3)	0.033 (3)	0.050 (4)	−0.002 (3)	0.018 (3)	−0.002 (3)
O11	0.040 (3)	0.042 (4)	0.046 (4)	0.003 (3)	0.015 (3)	0.007 (3)
O12	0.050 (4)	0.063 (4)	0.038 (4)	0.013 (3)	0.017 (3)	0.006 (3)
O13	0.047 (4)	0.049 (4)	0.050 (4)	−0.001 (3)	0.011 (3)	−0.007 (3)
N1	0.065 (6)	0.053 (6)	0.072 (6)	−0.011 (5)	0.011 (5)	0.000 (5)
N2	0.054 (4)	0.049 (4)	0.066 (4)	0.010 (3)	0.027 (4)	−0.001 (4)
C1	0.082 (9)	0.058 (8)	0.095 (10)	−0.017 (7)	0.019 (7)	0.000 (7)
C2	0.100 (11)	0.055 (9)	0.133 (13)	−0.013 (7)	0.020 (9)	−0.009 (8)
C3	0.169 (17)	0.053 (9)	0.121 (14)	−0.023 (10)	0.027 (12)	−0.004 (9)
C4	0.109 (12)	0.092 (12)	0.123 (13)	−0.048 (10)	−0.002 (9)	0.008 (10)
C5	0.082 (9)	0.081 (10)	0.080 (9)	−0.010 (7)	0.007 (7)	0.018 (7)
C6	0.066 (5)	0.055 (5)	0.093 (6)	−0.008 (4)	0.008 (4)	−0.003 (5)
C7	0.066 (4)	0.054 (4)	0.090 (5)	−0.005 (4)	0.004 (4)	0.001 (4)
C8	0.070 (4)	0.057 (4)	0.093 (5)	−0.002 (4)	0.004 (4)	0.003 (4)
C9	0.072 (4)	0.062 (4)	0.099 (5)	−0.003 (4)	0.002 (4)	0.005 (4)
C10	0.079 (5)	0.068 (5)	0.105 (5)	−0.005 (4)	0.001 (4)	0.007 (5)
C11	0.101 (5)	0.096 (5)	0.111 (5)	−0.003 (4)	0.001 (4)	0.006 (4)
C12	0.048 (6)	0.054 (7)	0.059 (7)	−0.002 (5)	0.020 (5)	−0.004 (5)
C13	0.052 (7)	0.058 (8)	0.094 (9)	0.011 (5)	0.022 (6)	0.007 (6)
C14	0.070 (8)	0.048 (7)	0.117 (11)	0.008 (6)	0.013 (7)	0.013 (7)
C15	0.077 (9)	0.104 (11)	0.099 (10)	0.013 (8)	0.047 (7)	0.051 (9)
C16	0.073 (8)	0.078 (9)	0.085 (9)	0.030 (7)	0.049 (7)	0.022 (7)
C17	0.064 (4)	0.053 (4)	0.070 (4)	0.007 (4)	0.024 (4)	−0.005 (4)
C18	0.071 (4)	0.060 (4)	0.078 (5)	0.005 (4)	0.024 (4)	−0.003 (4)
C19	0.081 (5)	0.065 (5)	0.079 (5)	0.002 (4)	0.026 (4)	−0.003 (4)
C20	0.091 (5)	0.077 (5)	0.086 (5)	0.003 (4)	0.025 (4)	−0.001 (4)
C21	0.102 (5)	0.086 (5)	0.091 (5)	0.005 (5)	0.026 (5)	0.004 (5)
C22	0.126 (5)	0.115 (5)	0.117 (5)	−0.002 (4)	0.014 (4)	0.003 (4)

Geometric parameters (Å, °)

Mo1—O1	1.672 (6)	C6—H6A	0.9700
Mo1—O2	1.694 (5)	C6—H6B	0.9700
Mo2—O3	1.678 (6)	C7—C8	1.496 (12)
Mo2—O4	1.684 (5)	C7—H7A	0.9700
Mo3—O5	1.684 (6)	C7—H7B	0.9700
Mo3—O6	1.692 (5)	C8—C9	1.504 (13)
Mo4—O7	1.686 (5)	C8—H8A	0.9700
Mo1—O9	1.867 (6)	C8—H8B	0.9700
Mo2—O12^{i}	1.925 (6)	C9—C10	1.510 (13)
Mo2—O9	1.926 (6)	C9—H9A	0.9700
Mo2—O13^{i}	2.311 (5)	C9—H9B	0.9700
Mo3—O12	1.870 (6)	C10—C11	1.501 (14)
Mo4—O13	1.725 (5)	C10—H10A	0.9700
Mo1—O11	1.989 (5)	C10—H10B	0.9700
Mo1—O8^{i}	2.295 (5)	C11—H11A	0.9600
Mo3—O8^{i}	1.976 (5)	C11—H11B	0.9600
Mo3—O11	2.311 (5)	C11—H11C	0.9600
Mo4—O11	1.939 (5)	C12—C13	1.355 (12)
Mo4—O8	1.951 (5)	C12—H12	0.9300
Mo2—O10	2.374 (5)	C13—C14	1.351 (13)
Mo1—O10	2.351 (5)	C13—H13	0.9300
Mo3—O10^{i}	2.344 (5)	C14—C15	1.367 (15)
Mo4—O10	2.128 (5)	C14—H14	0.9300
Mo4—O10^{i}	2.327 (5)	C15—C16	1.345 (15)
Mo1—Mo4	3.2085 (13)	C15—H15	0.9300
Mo1—Mo2	3.2154 (14)	C16—H16	0.9300
Mo3—Mo4^{i}	3.2188 (13)	C17—C18	1.481 (12)
Mo4—Mo3^{i}	3.2188 (13)	C17—H17A	0.9700
N1—C1	1.322 (12)	C17—H17B	0.9700
N1—C5	1.338 (13)	C18—C19	1.499 (13)
N1—C6	1.472 (12)	C18—H18A	0.9700
N2—C16	1.325 (10)	C18—H18B	0.9700
N2—C12	1.333 (10)	C19—C20	1.474 (13)
N2—C17	1.475 (11)	C19—H19A	0.9700
C1—C2	1.340 (14)	C19—H19B	0.9700
C1—H1	0.9300	C20—C21	1.547 (14)
C2—C3	1.342 (17)	C20—H20A	0.9700
C2—H2	0.9300	C20—H20B	0.9700
C3—C4	1.347 (17)	C21—C22	1.476 (15)
C3—H3	0.9300	C21—H21A	0.9700
C4—C5	1.362 (17)	C21—H21B	0.9700
C4—H4	0.9300	C22—H22A	0.9600
C5—H5	0.9300	C22—H22B	0.9600
C6—C7	1.507 (12)	C22—H22C	0.9600

O1—Mo1—O2	105.6 (3)	Mo4—O11—Mo3	110.7 (2)
O1—Mo1—O9	100.8 (3)	Mo1—O11—Mo3	102.8 (2)
O2—Mo1—O9	101.9 (3)	Mo3—O12—Mo2^{i}	116.3 (3)
O1—Mo1—O11	102.2 (3)	Mo4—O13—Mo2^{i}	115.7 (3)
O2—Mo1—O11	95.1 (2)	C1—N1—C5	121.6 (10)
O9—Mo1—O11	146.4 (2)	C1—N1—C6	117.7 (9)
O1—Mo1—O8^{i}	90.0 (2)	C5—N1—C6	120.6 (10)
O2—Mo1—O8^{i}	161.6 (2)	C16—N2—C12	121.2 (9)
O9—Mo1—O8^{i}	84.3 (2)	C16—N2—C17	120.2 (8)
O11—Mo1—O8^{i}	71.63 (19)	C12—N2—C17	118.5 (8)
O1—Mo1—O10	160.9 (2)	N1—C1—C2	121.0 (12)
O2—Mo1—O10	93.4 (2)	N1—C1—H1	119.5
O9—Mo1—O10	77.0 (2)	C2—C1—H1	119.5
O11—Mo1—O10	73.2 (2)	C1—C2—C3	118.8 (14)
O8^{i}—Mo1—O10	70.90 (17)	C1—C2—H2	120.6
O1—Mo1—Mo4	136.9 (2)	C3—C2—H2	120.6
O2—Mo1—Mo4	83.9 (2)	C2—C3—C4	120.3 (14)
O9—Mo1—Mo4	118.54 (17)	C2—C3—H3	119.9
O11—Mo1—Mo4	34.73 (15)	C4—C3—H3	119.9
O8^{i}—Mo1—Mo4	77.98 (13)	C3—C4—C5	120.4 (14)
O10—Mo1—Mo4	41.53 (13)	C3—C4—H4	119.8
O1—Mo1—Mo2	133.4 (2)	C5—C4—H4	119.8
O2—Mo1—Mo2	89.1 (2)	N1—C5—C4	117.8 (12)
O9—Mo1—Mo2	32.60 (17)	N1—C5—H5	121.1
O11—Mo1—Mo2	120.61 (16)	C4—C5—H5	121.1
O8^{i}—Mo1—Mo2	87.06 (14)	N1—C6—C7	112.8 (8)
O10—Mo1—Mo2	47.42 (13)	N1—C6—H6A	109.0
Mo4—Mo1—Mo2	87.65 (3)	C7—C6—H6A	109.0
O3—Mo2—O4	105.1 (3)	N1—C6—H6B	109.0
O3—Mo2—O12^{i}	101.6 (3)	C7—C6—H6B	109.0
O4—Mo2—O12^{i}	99.9 (3)	H6A—C6—H6B	107.8
O3—Mo2—O9	100.9 (3)	C8—C7—C6	110.3 (9)
O4—Mo2—O9	98.0 (3)	C8—C7—H7A	109.6
O12^{i}—Mo2—O9	146.4 (2)	C6—C7—H7A	109.6
O3—Mo2—O13^{i}	91.2 (2)	C8—C7—H7B	109.6
O4—Mo2—O13^{i}	163.7 (3)	C6—C7—H7B	109.6
O12^{i}—Mo2—O13^{i}	77.5 (2)	H7A—C7—H7B	108.1
O9—Mo2—O13^{i}	77.4 (2)	C7—C8—C9	113.9 (9)
O3—Mo2—O10	160.7 (2)	C7—C8—H8A	108.8
O4—Mo2—O10	94.2 (2)	C9—C8—H8A	108.8
O12^{i}—Mo2—O10	75.1 (2)	C7—C8—H8B	108.8
O9—Mo2—O10	75.4 (2)	C9—C8—H8B	108.8
O13^{i}—Mo2—O10	69.54 (18)	H8A—C8—H8B	107.7
O3—Mo2—Mo1	132.4 (2)	C8—C9—C10	112.0 (9)
O4—Mo2—Mo1	86.9 (2)	C8—C9—H9A	109.2

O12^{i}—Mo2—Mo1	121.87 (17)	C10—C9—H9A	109.2
O9—Mo2—Mo1	31.49 (17)	C8—C9—H9B	109.2
O13^{i}—Mo2—Mo1	81.13 (15)	C10—C9—H9B	109.2
O10—Mo2—Mo1	46.81 (13)	H9A—C9—H9B	107.9
O5—Mo3—O6	104.6 (3)	C11—C10—C9	112.1 (10)
O5—Mo3—O12	101.6 (3)	C11—C10—H10A	109.2
O6—Mo3—O12	101.6 (3)	C9—C10—H10A	109.2
O5—Mo3—O8^{i}	101.9 (3)	C11—C10—H10B	109.2
O6—Mo3—O8^{i}	96.3 (3)	C9—C10—H10B	109.2
O12—Mo3—O8^{i}	145.7 (2)	H10A—C10—H10B	107.9
O5—Mo3—O11	89.2 (2)	C10—C11—H11A	109.5
O6—Mo3—O11	163.4 (2)	C10—C11—H11B	109.5
O12—Mo3—O11	84.3 (2)	H11A—C11—H11B	109.5
O8^{i}—Mo3—O11	71.48 (19)	C10—C11—H11C	109.5
O5—Mo3—O10^{i}	160.5 (2)	H11A—C11—H11C	109.5
O6—Mo3—O10^{i}	94.7 (2)	H11B—C11—H11C	109.5
O12—Mo3—O10^{i}	76.8 (2)	N2—C12—C13	120.1 (9)
O8^{i}—Mo3—O10^{i}	72.70 (19)	N2—C12—H12	119.9
O11—Mo3—O10^{i}	71.27 (18)	C13—C12—H12	119.9
O5—Mo3—Mo4^{i}	136.5 (2)	C14—C13—C12	119.2 (10)
O6—Mo3—Mo4^{i}	85.0 (2)	C14—C13—H13	120.4
O12—Mo3—Mo4^{i}	118.11 (17)	C12—C13—H13	120.4
O8^{i}—Mo3—Mo4^{i}	34.68 (15)	C13—C14—C15	119.7 (11)
O11—Mo3—Mo4^{i}	78.62 (13)	C13—C14—H14	120.2
O10^{i}—Mo3—Mo4^{i}	41.35 (13)	C15—C14—H14	120.2
O7—Mo4—O13	105.1 (3)	C16—C15—C14	119.6 (10)
O7—Mo4—O11	102.0 (2)	C16—C15—H15	120.2
O13—Mo4—O11	96.5 (2)	C14—C15—H15	120.2
O7—Mo4—O8	100.1 (2)	N2—C16—C15	120.0 (10)
O13—Mo4—O8	96.5 (2)	N2—C16—H16	120.0
O11—Mo4—O8	150.4 (2)	C15—C16—H16	120.0
O7—Mo4—O10	97.8 (2)	N2—C17—C18	113.2 (8)
O13—Mo4—O10	157.1 (2)	N2—C17—H17A	108.9
O11—Mo4—O10	79.4 (2)	C18—C17—H17A	108.9
O8—Mo4—O10	78.3 (2)	N2—C17—H17B	108.9
O7—Mo4—O10^{i}	173.7 (2)	C18—C17—H17B	108.9
O13—Mo4—O10^{i}	81.1 (2)	H17A—C17—H17B	107.8
O11—Mo4—O10^{i}	78.36 (19)	C17—C18—C19	113.5 (9)
O8—Mo4—O10^{i}	77.54 (19)	C17—C18—H18A	108.9
O10—Mo4—O10^{i}	76.0 (2)	C19—C18—H18A	108.9
O7—Mo4—Mo1	90.55 (19)	C17—C18—H18B	108.9
O13—Mo4—Mo1	132.26 (19)	C19—C18—H18B	108.9
O11—Mo4—Mo1	35.74 (16)	H18A—C18—H18B	107.7
O8—Mo4—Mo1	125.31 (16)	C20—C19—C18	115.2 (9)

O10—Mo4—Mo1	47.10 (14)	C20—C19—H19A	108.5
O10^{i}—Mo4—Mo1	86.19 (13)	C18—C19—H19A	108.5
O7—Mo4—Mo3^{i}	88.7 (2)	C20—C19—H19B	108.5
O13—Mo4—Mo3^{i}	131.65 (19)	C18—C19—H19B	108.5
O11—Mo4—Mo3^{i}	126.12 (16)	H19A—C19—H19B	107.5
O8—Mo4—Mo3^{i}	35.19 (15)	C19—C20—C21	111.9 (10)
O10—Mo4—Mo3^{i}	46.69 (14)	C19—C20—H20A	109.2
O10^{i}—Mo4—Mo3^{i}	86.06 (13)	C21—C20—H20A	109.2
Mo1—Mo4—Mo3^{i}	92.62 (3)	C19—C20—H20B	109.2
Mo4—O8—Mo3^{i}	110.1 (2)	C21—C20—H20B	109.2
Mo4—O8—Mo1^{i}	111.4 (2)	H20A—C20—H20B	107.9
Mo3^{i}—O8—Mo1^{i}	103.8 (2)	C22—C21—C20	111.6 (11)
Mo1—O9—Mo2	115.9 (3)	C22—C21—H21A	109.3
Mo4—O10—Mo4^{i}	104.0 (2)	C20—C21—H21A	109.3
Mo4—O10—Mo3^{i}	91.96 (19)	C22—C21—H21B	109.3
Mo4^{i}—O10—Mo3^{i}	97.19 (19)	C20—C21—H21B	109.3
Mo4—O10—Mo1	91.4 (2)	H21A—C21—H21B	108.0
Mo4^{i}—O10—Mo1	97.37 (18)	C21—C22—H22A	109.5
Mo3^{i}—O10—Mo1	163.8 (2)	C21—C22—H22B	109.5
Mo4—O10—Mo2	162.3 (2)	H22A—C22—H22B	109.5
Mo4^{i}—O10—Mo2	93.72 (19)	C21—C22—H22C	109.5
Mo3^{i}—O10—Mo2	86.24 (18)	H22A—C22—H22C	109.5
Mo1—O10—Mo2	85.76 (17)	H22B—C22—H22C	109.5
Mo4—O11—Mo1	109.5 (2)		
O1—Mo1—Mo2—O3	−0.1 (4)	O8—Mo4—O10—Mo2	−101.8 (9)
O2—Mo1—Mo2—O3	−110.9 (3)	O10^{i}—Mo4—O10—Mo2	178.3 (10)
O9—Mo1—Mo2—O3	3.0 (4)	Mo1—Mo4—O10—Mo2	80.4 (8)
O11—Mo1—Mo2—O3	153.7 (3)	Mo3^{i}—Mo4—O10—Mo2	−83.8 (8)
O8^{i}—Mo1—Mo2—O3	87.1 (3)	O1—Mo1—O10—Mo4	−96.1 (8)
O10—Mo1—Mo2—O3	153.6 (3)	O2—Mo1—O10—Mo4	76.8 (2)
Mo4—Mo1—Mo2—O3	165.2 (3)	O9—Mo1—O10—Mo4	178.2 (2)
O1—Mo1—Mo2—O4	107.6 (3)	O11—Mo1—O10—Mo4	−17.47 (18)
O2—Mo1—Mo2—O4	−3.2 (3)	O8^{i}—Mo1—O10—Mo4	−93.4 (2)
O9—Mo1—Mo2—O4	110.7 (4)	Mo2—Mo1—O10—Mo4	162.5 (2)
O11—Mo1—Mo2—O4	−98.6 (3)	O1—Mo1—O10—Mo4^{i}	8.2 (9)
O8^{i}—Mo1—Mo2—O4	−165.2 (2)	O2—Mo1—O10—Mo4^{i}	−178.9 (2)
O10—Mo1—Mo2—O4	−98.7 (3)	O9—Mo1—O10—Mo4^{i}	−77.5 (2)
Mo4—Mo1—Mo2—O4	−87.1 (2)	O11—Mo1—O10—Mo4^{i}	86.8 (2)
O1—Mo1—Mo2—O12^{i}	−152.7 (3)	O8^{i}—Mo1—O10—Mo4^{i}	10.94 (18)
O2—Mo1—Mo2—O12^{i}	96.5 (3)	Mo4—Mo1—O10—Mo4^{i}	104.3 (2)
O9—Mo1—Mo2—O12^{i}	−149.6 (4)	Mo2—Mo1—O10—Mo4^{i}	−93.2 (2)
O11—Mo1—Mo2—O12^{i}	1.1 (3)	O1—Mo1—O10—Mo3^{i}	162.0 (9)

O8^{i}—Mo1—Mo2—O12^{i}	−65.6 (2)	O2—Mo1—O10—Mo3^{i}	−25.0 (10)
O10—Mo1—Mo2—O12^{i}	1.0 (2)	O9—Mo1—O10—Mo3^{i}	76.4 (10)
Mo4—Mo1—Mo2—O12^{i}	12.53 (19)	O11—Mo1—O10—Mo3^{i}	−119.3 (10)
O1—Mo1—Mo2—O9	−3.2 (4)	O8^{i}—Mo1—O10—Mo3^{i}	164.8 (10)
O2—Mo1—Mo2—O9	−114.0 (4)	Mo4—Mo1—O10—Mo3^{i}	−101.9 (10)
O11—Mo1—Mo2—O9	150.7 (3)	Mo2—Mo1—O10—Mo3^{i}	60.6 (9)
O8^{i}—Mo1—Mo2—O9	84.0 (3)	O1—Mo1—O10—Mo2	101.4 (8)
O10—Mo1—Mo2—O9	150.6 (3)	O2—Mo1—O10—Mo2	−85.7 (2)
Mo4—Mo1—Mo2—O9	162.1 (3)	O9—Mo1—O10—Mo2	15.75 (18)
O1—Mo1—Mo2—O13^{i}	−83.5 (3)	O11—Mo1—O10—Mo2	−180.0 (2)
O2—Mo1—Mo2—O13^{i}	165.7 (2)	O8^{i}—Mo1—O10—Mo2	104.2 (2)
O9—Mo1—Mo2—O13^{i}	−80.4 (3)	Mo4—Mo1—O10—Mo2	−162.5 (2)
O11—Mo1—Mo2—O13^{i}	70.3 (2)	O3—Mo2—O10—Mo4	−177.9 (8)
O8^{i}—Mo1—Mo2—O13^{i}	3.65 (19)	O4—Mo2—O10—Mo4	0.6 (9)
O10—Mo1—Mo2—O13^{i}	70.2 (2)	O12^{i}—Mo2—O10—Mo4	99.7 (9)
Mo4—Mo1—Mo2—O13^{i}	81.73 (14)	O9—Mo2—O10—Mo4	−96.6 (9)
O1—Mo1—Mo2—O10	−153.8 (3)	O13^{i}—Mo2—O10—Mo4	−178.4 (9)
O2—Mo1—Mo2—O10	95.4 (3)	Mo1—Mo2—O10—Mo4	−81.2 (8)
O9—Mo1—Mo2—O10	−150.6 (3)	O3—Mo2—O10—Mo4^{i}	0.5 (9)
O11—Mo1—Mo2—O10	0.1 (2)	O4—Mo2—O10—Mo4^{i}	178.9 (2)
O8^{i}—Mo1—Mo2—O10	−66.6 (2)	O12^{i}—Mo2—O10—Mo4^{i}	−82.0 (2)
Mo4—Mo1—Mo2—O10	11.52 (16)	O9—Mo2—O10—Mo4^{i}	81.8 (2)
O1—Mo1—Mo4—O7	−108.3 (4)	O13^{i}—Mo2—O10—Mo4^{i}	−0.02 (17)
O2—Mo1—Mo4—O7	−2.0 (3)	Mo1—Mo2—O10—Mo4^{i}	97.12 (18)
O9—Mo1—Mo4—O7	98.2 (3)	O3—Mo2—O10—Mo3^{i}	97.4 (8)
O11—Mo1—Mo4—O7	−110.1 (3)	O4—Mo2—O10—Mo3^{i}	−84.1 (2)
O8^{i}—Mo1—Mo4—O7	174.9 (2)	O12^{i}—Mo2—O10—Mo3^{i}	14.98 (19)
O10—Mo1—Mo4—O7	100.2 (3)	O9—Mo2—O10—Mo3^{i}	178.7 (2)
Mo2—Mo1—Mo4—O7	87.4 (2)	O13^{i}—Mo2—O10—Mo3^{i}	97.0 (2)
O1—Mo1—Mo4—O13	2.8 (4)	Mo1—Mo2—O10—Mo3^{i}	−165.9 (2)
O2—Mo1—Mo4—O13	109.1 (3)	O3—Mo2—O10—Mo1	−96.7 (8)
O9—Mo1—Mo4—O13	−150.6 (3)	O4—Mo2—O10—Mo1	81.8 (2)
O11—Mo1—Mo4—O13	1.0 (3)	O12^{i}—Mo2—O10—Mo1	−179.1 (2)
O8^{i}—Mo1—Mo4—O13	−74.0 (3)	O9—Mo2—O10—Mo1	−15.36 (18)
O10—Mo1—Mo4—O13	−148.7 (3)	O13^{i}—Mo2—O10—Mo1	−97.14 (19)
Mo2—Mo1—Mo4—O13	−161.5 (2)	O7—Mo4—O11—Mo1	73.8 (3)
O1—Mo1—Mo4—O11	1.8 (4)	O13—Mo4—O11—Mo1	−179.2 (3)
O2—Mo1—Mo4—O11	108.1 (3)	O8—Mo4—O11—Mo1	−63.7 (5)
O9—Mo1—Mo4—O11	−151.7 (3)	O10—Mo4—O11—Mo1	−22.1 (2)
O8^{i}—Mo1—Mo4—O11	−75.0 (3)	O10^{i}—Mo4—O11—Mo1	−99.8 (3)
O10—Mo1—Mo4—O11	−149.7 (3)	Mo3^{i}—Mo4—O11—Mo1	−23.5 (3)
Mo2—Mo1—Mo4—O11	−162.5 (2)	O7—Mo4—O11—Mo3	−173.5 (3)

O1—Mo1—Mo4—O8	148.9 (3)	O13—Mo4—O11—Mo3	−66.6 (3)
O2—Mo1—Mo4—O8	−104.8 (3)	O8—Mo4—O11—Mo3	48.9 (5)
O9—Mo1—Mo4—O8	−4.5 (3)	O10—Mo4—O11—Mo3	90.6 (2)
O11—Mo1—Mo4—O8	147.1 (3)	$O10^{i}$—Mo4—O11—Mo3	12.9 (2)
$O8^{i}$—Mo1—Mo4—O8	72.1 (2)	Mo1—Mo4—O11—Mo3	112.7 (3)
O10—Mo1—Mo4—O8	−2.6 (2)	$Mo3^{i}$—Mo4—O11—Mo3	89.2 (2)
Mo2—Mo1—Mo4—O8	−15.39 (17)	O1—Mo1—O11—Mo4	−178.8 (3)
O1—Mo1—Mo4—O10	151.5 (4)	O2—Mo1—O11—Mo4	−71.6 (3)
O2—Mo1—Mo4—O10	−102.2 (3)	O9—Mo1—O11—Mo4	48.9 (5)
O9—Mo1—Mo4—O10	−2.0 (3)	$O8^{i}$—Mo1—O11—Mo4	95.4 (3)
O11—Mo1—Mo4—O10	149.7 (3)	O10—Mo1—O11—Mo4	20.4 (2)
$O8^{i}$—Mo1—Mo4—O10	74.7 (2)	Mo2—Mo1—O11—Mo4	20.4 (3)
Mo2—Mo1—Mo4—O10	−12.82 (18)	O1—Mo1—O11—Mo3	63.5 (3)
O1—Mo1—Mo4—$O10^{i}$	77.1 (3)	O2—Mo1—O11—Mo3	170.7 (2)
O2—Mo1—Mo4—$O10^{i}$	−176.6 (2)	O9—Mo1—O11—Mo3	−68.8 (5)
O9—Mo1—Mo4—$O10^{i}$	−76.4 (2)	$O8^{i}$—Mo1—O11—Mo3	−22.35 (18)
O11—Mo1—Mo4—$O10^{i}$	75.3 (3)	O10—Mo1—O11—Mo3	−97.3 (2)
$O8^{i}$—Mo1—Mo4—$O10^{i}$	0.28 (19)	Mo4—Mo1—O11—Mo3	−117.7 (3)
O10—Mo1—Mo4—$O10^{i}$	−74.4 (2)	Mo2—Mo1—O11—Mo3	−97.32 (18)
Mo2—Mo1—Mo4—$O10^{i}$	−87.21 (14)	O5—Mo3—O11—Mo4	166.5 (3)
O1—Mo1—Mo4—$Mo3^{i}$	163.0 (3)	O6—Mo3—O11—Mo4	−46.8 (10)
O2—Mo1—Mo4—$Mo3^{i}$	−90.7 (2)	O12—Mo3—O11—Mo4	64.7 (3)
O9—Mo1—Mo4—$Mo3^{i}$	9.51 (18)	$O8^{i}$—Mo3—O11—Mo4	−90.7 (3)
O11—Mo1—Mo4—$Mo3^{i}$	161.2 (2)	$O10^{i}$—Mo3—O11—Mo4	−13.2 (2)
$O8^{i}$—Mo1—Mo4—$Mo3^{i}$	86.15 (14)	$Mo4^{i}$—Mo3—O11—Mo4	−55.5 (2)
O10—Mo1—Mo4—$Mo3^{i}$	11.47 (18)	O5—Mo3—O11—Mo1	−76.6 (3)
Mo2—Mo1—Mo4—$Mo3^{i}$	−1.34 (3)	O6—Mo3—O11—Mo1	70.1 (9)
O7—Mo4—O8—$Mo3^{i}$	−73.0 (3)	O12—Mo3—O11—Mo1	−178.4 (3)
O13—Mo4—O8—$Mo3^{i}$	−179.7 (3)	$O8^{i}$—Mo3—O11—Mo1	26.2 (2)
O11—Mo4—O8—$Mo3^{i}$	64.8 (5)	$O10^{i}$—Mo3—O11—Mo1	103.7 (2)
O10—Mo4—O8—$Mo3^{i}$	23.0 (2)	$Mo4^{i}$—Mo3—O11—Mo1	61.42 (18)
$O10^{i}$—Mo4—O8—$Mo3^{i}$	101.0 (3)	O5—Mo3—O12—$Mo2^{i}$	178.7 (3)
Mo1—Mo4—O8—$Mo3^{i}$	24.9 (3)	O6—Mo3—O12—$Mo2^{i}$	70.9 (3)
O7—Mo4—O8—$Mo1^{i}$	172.3 (3)	$O8^{i}$—Mo3—O12—$Mo2^{i}$	−48.9 (5)
O13—Mo4—O8—$Mo1^{i}$	65.7 (3)	O11—Mo3—O12—$Mo2^{i}$	−93.3 (3)
O11—Mo4—O8—$Mo1^{i}$	−49.8 (5)	$O10^{i}$—Mo3—O12—$Mo2^{i}$	−21.3 (2)
O10—Mo4—O8—$Mo1^{i}$	−91.7 (2)	$Mo4^{i}$—Mo3—O12—$Mo2^{i}$	−19.5 (3)
$O10^{i}$—Mo4—O8—$Mo1^{i}$	−13.6 (2)	O7—Mo4—O13—$Mo2^{i}$	−178.5 (3)
Mo1—Mo4—O8—$Mo1^{i}$	−89.8 (2)	O11—Mo4—O13—$Mo2^{i}$	77.1 (3)
$Mo3^{i}$—Mo4—O8—$Mo1^{i}$	−114.7 (4)	O8—Mo4—O13—$Mo2^{i}$	−76.2 (3)
O1—Mo1—O9—Mo2	177.7 (3)	O10—Mo4—O13—$Mo2^{i}$	−1.2 (8)
O2—Mo1—O9—Mo2	69.0 (3)	$O10^{i}$—Mo4—O13—$Mo2^{i}$	0.0 (3)

O11—Mo1—O9—Mo2	−49.7 (5)	Mo1—Mo4—O13—Mo2^{i}	76.5 (3)
O8^{i}—Mo1—O9—Mo2	−93.4 (3)	Mo3^{i}—Mo4—O13—Mo2^{i}	−76.5 (3)
O10—Mo1—O9—Mo2	−21.8 (2)	C5—N1—C1—C2	−1.2 (17)
Mo4—Mo1—O9—Mo2	−20.4 (3)	C6—N1—C1—C2	175.2 (10)
O3—Mo2—O9—Mo1	−177.7 (3)	N1—C1—C2—C3	1(2)
O4—Mo2—O9—Mo1	−70.6 (3)	C1—C2—C3—C4	−1(2)
O12^{i}—Mo2—O9—Mo1	50.9 (6)	C2—C3—C4—C5	1(2)
O13^{i}—Mo2—O9—Mo1	93.5 (3)	C1—N1—C5—C4	1.9 (17)
O10—Mo2—O9—Mo1	21.7 (2)	C6—N1—C5—C4	−174.4 (10)
O7—Mo4—O10—Mo4^{i}	178.6 (2)	C3—C4—C5—N1	−2(2)
O13—Mo4—O10—Mo4^{i}	1.3 (7)	C1—N1—C6—C7	−80.5 (12)
O11—Mo4—O10—Mo4^{i}	−80.5 (2)	C5—N1—C6—C7	95.9 (11)
O8—Mo4—O10—Mo4^{i}	79.9 (2)	N1—C6—C7—C8	172.8 (9)
O10^{i}—Mo4—O10—Mo4^{i}	0.0	C6—C7—C8—C9	−176.4 (9)
Mo1—Mo4—O10—Mo4^{i}	−97.9 (2)	C7—C8—C9—C10	−179.9 (9)
Mo3^{i}—Mo4—O10—Mo4^{i}	97.9 (2)	C8—C9—C10—C11	179.9 (10)
O7—Mo4—O10—Mo3^{i}	80.7 (2)	C16—N2—C12—C13	−1.7 (15)
O13—Mo4—O10—Mo3^{i}	−96.7 (6)	C17—N2—C12—C13	−178.0 (9)
O11—Mo4—O10—Mo3^{i}	−178.4 (2)	N2—C12—C13—C14	2.3 (16)
O8—Mo4—O10—Mo3^{i}	−18.00 (17)	C12—C13—C14—C15	−4.0 (17)
O10^{i}—Mo4—O10—Mo3^{i}	−97.9 (2)	C13—C14—C15—C16	5.1 (19)
Mo1—Mo4—O10—Mo3^{i}	164.2 (2)	C12—N2—C16—C15	2.7 (17)
O7—Mo4—O10—Mo1	−83.4 (2)	C17—N2—C16—C15	179.0 (10)
O13—Mo4—O10—Mo1	99.2 (6)	C14—C15—C16—N2	−4.4 (19)
O11—Mo4—O10—Mo1	17.44 (17)	C16—N2—C17—C18	−93.2 (11)
O8—Mo4—O10—Mo1	177.9 (2)	C12—N2—C17—C18	83.2 (10)
O10^{i}—Mo4—O10—Mo1	97.9 (2)	N2—C17—C18—C19	−170.0 (8)
Mo3^{i}—Mo4—O10—Mo1	−164.2 (2)	C17—C18—C19—C20	−176.7 (9)
O7—Mo4—O10—Mo2	−3.1 (9)	C18—C19—C20—C21	−179.2 (9)
O13—Mo4—O10—Mo2	179.6 (7)	C19—C20—C21—C22	−173.3 (10)
O11—Mo4—O10—Mo2	97.8 (9)		

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

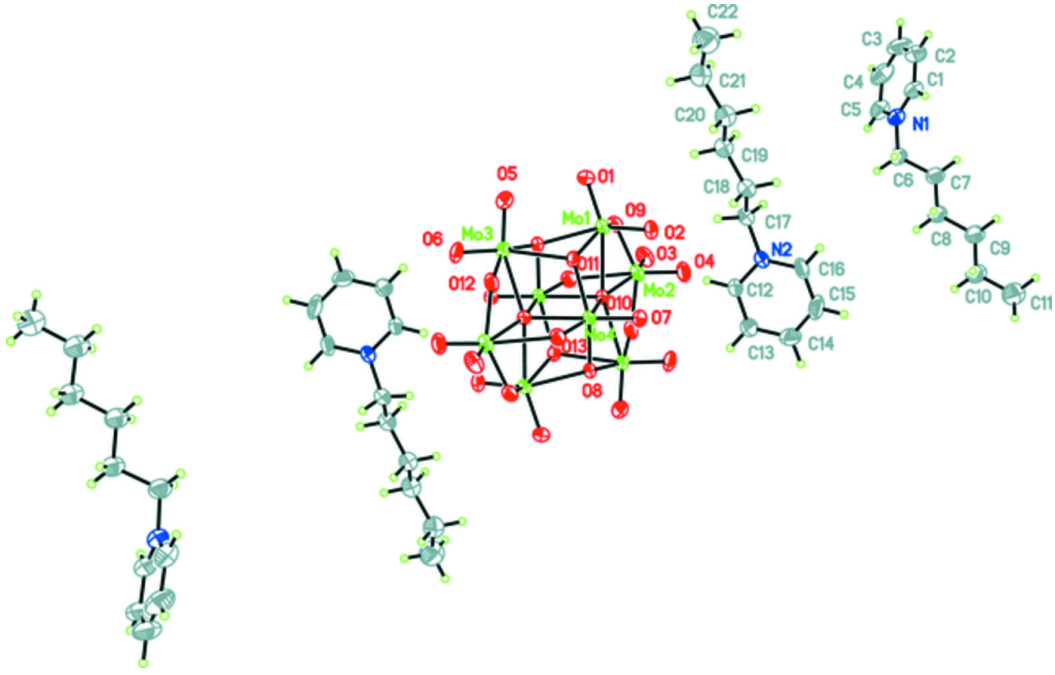
Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19A···O4^{ii}	0.97	2.60	3.391 (12)	139
C17—H17B···O6^{iii}	0.97	2.30	3.200 (11)	154
C17—H17A···O4	0.97	2.48	3.207 (11)	131
C17—H17A···O2	0.97	2.46	3.166 (10)	130
C16—H16···O5^{iii}	0.93	2.40	3.271 (11)	155
C15—H15···O9^{iv}	0.93	2.56	3.257 (13)	132
C12—H12···O2	0.93	2.40	3.243 (11)	151
C7—H7B···O3^{iii}	0.97	2.40	3.143 (12)	133

C5—H5···O1^{v}	0.93	2.39	3.059 (13)	129
C4—H4···O8^{vi}	0.93	2.56	3.295 (15)	136
C1—H1···O3^{iii}	0.93	2.50	3.295 (13)	144

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

Fig. 1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C9
C10
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Mo3
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04
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Mo2
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Mo4
013
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Fig. 2