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Bis(1,10-phenanthroline-κ^2N,N')-copper(I) chloridobis(1,10-phenanthroline-κ^2N,N')copper(II) hexacosaoxidooctamolybdate(VI) dihydrate

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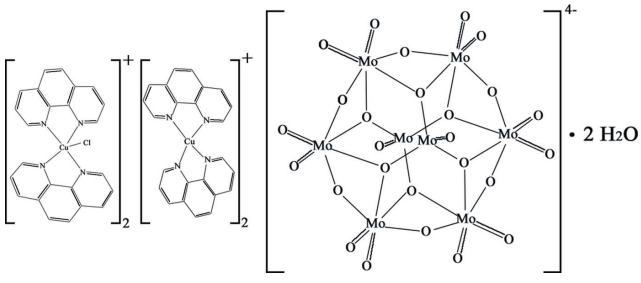
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; R factor = 0.032; wR factor = 0.072; data-to-parameter ratio = 13.9.

The title complex, $[Cu^{II}Cl(C_{12}H_8N_2)_2]_2[Cu^{I}(C_{12}H_8N_2)_2]_2[Mo_8O_{26}]\cdot 2H_2O$, features a centrosymmetric α-type octamolybdate anion, two complex copper counter-cations with Cu in oxidation states +II and +I, and two water molecules of crystallization. The Cu^{II} ion exhibits a distorted CuN_4Cl square-pyramidal coordination, whereas the Cu^{I} ion is in a distorted tetrahedral CuN_4 coordination. The anions, cations and uncoordinated water molecules are linked into a three-dimensional network by O—H···O and C—H···O hydrogen bonds.

Related literature

For recent studies of other polyoxomolybdates, see Allis *et al.* (2004). The bond-valence sums (BVS) were calculated according to Brown & Altermatt (1985).



Experimental

Crystal data

$[CuCl(C_{12}H_8N_2)_2]_2[Cu(C_{12}H_8N_2)_2]_2[Mo_8O_{26}]\cdot 2H_2O$
M_r = 2986.29
Triclinic, $P\overline{1}$
a = 12.442 (2) Å
b = 13.604 (2) Å
c = 14.902 (3) Å
α = 101.115 (4)°
β = 91.514 (3)°
γ = 95.880 (3)°
V = 2459.2 (7) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 1.97 mm^{-1}
T = 295 (2) K
0.21 × 0.20 × 0.12 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.665, T_{max} = 0.780
21242 measured reflections
9614 independent reflections
7435 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.072
S = 1.05
9614 reflections
694 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.41 e Å^{-3}
$\Delta\rho_{min}$ = −0.61 e Å^{-3}

Table 1
Selected bond lengths (Å).

Mo1—O1	1.701 (2)	Mo3—O6	2.499 (3)
Mo1—O9^{i}	1.784 (2)	Mo4—O13	1.694 (3)
Mo1—O6	1.786 (3)	Mo4—O11	1.703 (3)
Mo1—O3	1.790 (2)	Mo4—O2	1.891 (2)
Mo2—O7	1.693 (3)	Mo4—O4	1.905 (2)
Mo2—O8	1.695 (2)	Mo4—O3	2.410 (2)
Mo2—O4	1.908 (2)	Cu1—N5	1.984 (3)
Mo2—O10^{i}	1.924 (2)	Cu1—N2	1.992 (3)
Mo2—O6^{i}	2.354 (3)	Cu1—N1	2.075 (3)
Mo2—O3	2.424 (2)	Cu1—N3	2.177 (3)
Mo3—O12	1.692 (2)	Cu1—Cl	2.2750 (12)
Mo3—O5	1.692 (3)	Cu2—N8	2.025 (3)
Mo3—O10	1.905 (3)	Cu2—N4	2.028 (3)
Mo3—O2	1.917 (3)	Cu2—N6	2.044 (4)
Mo3—O9	2.380 (2)	Cu2—N7	2.047 (4)

Symmetry code: (i) $-x+1, -y, -z+1$.

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

D—H···A	D—H	H···A	D···A	D—H···A
OW—H1W···O7^{ii}	0.93	2.52	3.074 (6)	119
OW—H1W···O10^{iii}	0.93	2.15	3.005 (6)	152
C11—H11···O8^{i}	0.93	2.40	3.215 (5)	146
C12—H12···O8^{iv}	0.93	2.49	3.295 (5)	145
C16—H16···O7^{v}	0.93	2.41	3.320 (5)	166
C20—H20···O12	0.93	2.40	3.049 (5)	127
C22—H22···O1^{v}	0.93	2.53	3.213 (5)	131
C24—H24···O13^{vi}	0.93	2.41	3.164 (6)	138
C25—H25···O11^{iii}	0.93	2.41	3.301 (5)	161
C26—H26···O4^{iii}	0.93	2.58	3.327 (4)	137
C38—H38···OW	0.93	2.59	3.328 (6)	137
C40—H40···O2^{ii}	0.93	2.39	3.273 (5)	159

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

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: WM2120).

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supplementary materials

Acta Cryst. (2007). E**63**, m1993-m1994 [**doi:10.1107/S1600536807030450**]

Bis(1,10-phenanthroline-κ^2N,N')copper(I) chloridobis(1,10-phenanthroline-κ^2N,N')copper(II) hexacosaoxidooctamolybdate(VI) dihydrate

W.-J. Wang and L. Xu

Comment

Recently, polyoxomolybdates (POM) containing transition-metal complexes have been extensively investigated (Allis *et al.*, 2004). Among the syntheses of these inorganic-organic hybrids, the hydrothermal method is an effective method. To further explore this synthetic approach for new POM structures, the title complex, (I), is reported here.

The structure of complex (I) contains a $[Mo_8O_{26}]^{4-}$ anion, two $[Cu^{II}(phen)_2Cl]^+$ and $[Cu^{I}(phen)_2]^+$ (phen = 1,10-phenanthroline) counter cations, and isolated water molecules. The centrosymmetric $[Mo_8O_{26}]^{4-}$ cluster (Fig. 1) is of the α-type and is made up of a ring of six edge-sharing MoO_6 octahedra, bicapped by two *trans*-MoO_4 tetrahedra. In the $[Cu^{II}(phen)_2Cl]^+$ complex cation, $Cu1^{II}$ exhibits a distorted CuN_4Cl square-pyramidal coordination to four N atoms from two phen ligands and to one Cl atom. The $Cu2^{I}$ cation in the $[Cu^{I}(phen)_2]^+$ complex is coordinated by four N atoms from two phen ligands forming a considerably distorted CuN_4 tetrahedron. The Mo—O, Cu—N, and Cu—Cl distances are in the range 1.692 (2) to 2.499 (3) Å, 1.984 (3) to 2.177 (3) Å, and 2.2750 (12) Å, respectively. Bond valence sum (BVS) calculations (Brown & Altermatt, 1985) are close to the expected oxidation states, with 5.95 to 6.07 valence units (v.u.) for the Mo atoms (expected 6), 2.25 v.u. for $Cu1^{II}$ (expected 2), and 0.99 for $Cu2^{I}$ (expected 1).

Hydrogen bonding (Table 2) of the type O—H···O and C—H···O between the anions, cations, and the isolated water molecules consolidates the structure into a three-dimensional framework, as shown in Fig. 2.

Experimental

All employed reagents were purchased from Shanghai Reagent Company with analytical purity. $Na_2MoO_4{\cdot}2H_2O$ (1 g, 4.1 mmol), $Cu(CH_3COO)_2{\cdot}2H_2O$ (0.1 g, 0.5 mmol), and phen (0.4 g, 2 mmol) were dissolved in 10 ml 0.2 *M* HCl under stirring. The suspension was then placed in a 20-ml Teflon-lined reactor. After heating the mixture for 7 d at 413 K, blue block-like crystals of (I) were obtained.

Refinement

The aromatic H atoms were placed at calculated positions (C—H = 0.93 Å) and were allowed to ride on their carrier atoms with $U(H)_{iso}$=1.2$U(C)_{eq}$. The H atoms of the water molecules were located in difference Fourier maps and refined in their as-found relative positions with distances between 0.86–0.93 Å using a riding model with $U(H)_{iso}$ = 1.2$U(O)_{eq}$.

Figures

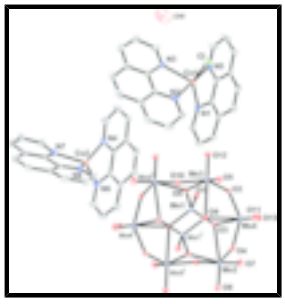


Fig. 1. The cationic and anionic moieties of (I). Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) $1-x, -y, 1-z$.]

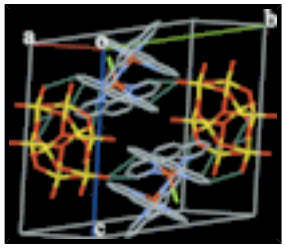


Fig. 2. The unit cell packing of (I).

Bis(1,10-phenanthroline-κ^2N,N')copper(I) chloridobis(1,10-phenanthroline-κ^2N,N')copper(II) hexacosaoxidooctamolybdate(VI) dihydrate

Crystal data

$[CuCl(C_{12}H_8N_2)_2]_2[Cu(C_{12}H_8N_2)_2]_2[Mo_8O_{26}]\cdot 2H_2O$	$Z = 1$
$M_r = 2986.29$	$F_{000} = 1466$
Triclinic, $P\overline{1}$	$D_x = 2.016$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 12.442$ (2) Å	Cell parameters from 13762 reflections
$b = 13.604$ (2) Å	$\theta = 1.8$–27.5°
$c = 14.902$ (3) Å	$\mu = 1.97$ mm^{-1}
$\alpha = 101.115$ (4)°	$T = 295$ (2) K
$\beta = 91.514$ (3)°	Block, blue
$\gamma = 95.880$ (3)°	0.21 × 0.20 × 0.12 mm
$V = 2459.2$ (7) Å^3	

Data collection

Bruker SMART CCD APEXII diffractometer	9614 independent reflections
Radiation source: fine-focus sealed tube	7435 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.038$
$T = 295$(2) K	$\theta_{max} = 26.0^\circ$
ω and φ scans	$\theta_{min} = 3.1^\circ$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$h = -15\rightarrow 15$

T_{min} = 0.665, T_{max} = 0.780	k = −16→16
21242 measured reflections	l = −18→18

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.032	H-atom parameters constrained
$wR(F^2)$ = 0.072	$w = 1/[\sigma^2(F_o^2) + (0.0315P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max} < 0.001$
9614 reflections	$\Delta\rho_{max}$ = 0.41 e Å^{-3}
694 parameters	$\Delta\rho_{min}$ = −0.61 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 $F^2 > \sigma(F^2)$ 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	0.55938 (2)	0.120262 (19)	0.47442 (2)	0.02134 (8)
Mo2	0.74571 (3)	−0.07803 (2)	0.51262 (2)	0.02540 (8)
Mo3	0.39186 (3)	0.11660 (2)	0.69193 (2)	0.02685 (8)
Mo4	0.64840 (3)	0.05475 (2)	0.70119 (2)	0.02548 (8)
Cu1	0.18668 (4)	0.53747 (3)	0.73391 (3)	0.02875 (11)
Cu2	0.21367 (5)	0.27923 (4)	0.09753 (4)	0.04924 (15)
Cl	0.11512 (10)	0.56271 (8)	0.87436 (8)	0.0495 (3)
O1	0.6114 (2)	0.23538 (17)	0.45726 (19)	0.0366 (7)
O2	0.5459 (2)	0.14846 (16)	0.70242 (17)	0.0288 (6)
O3	0.6537 (2)	0.07276 (16)	0.54355 (16)	0.0275 (6)
O4	0.6891 (2)	−0.06733 (16)	0.63143 (16)	0.0265 (5)
O5	0.3618 (2)	0.07120 (18)	0.78738 (18)	0.0384 (7)
O6	0.4365 (2)	0.13368 (17)	0.53276 (17)	0.0302 (6)
O7	0.8682 (2)	−0.0108 (2)	0.5401 (2)	0.0426 (7)
O8	0.7720 (2)	−0.19996 (18)	0.49288 (19)	0.0397 (7)
O9	0.4689 (2)	−0.03415 (16)	0.63208 (17)	0.0288 (6)

O10	0.2756 (2)	0.05199 (17)	0.60866 (17)	0.0294 (6)
O11	0.6279 (2)	0.01793 (19)	0.80289 (18)	0.0377 (7)
O12	0.3585 (2)	0.23607 (17)	0.7153 (2)	0.0402 (7)
O13	0.7656 (2)	0.13251 (19)	0.71968 (19)	0.0390 (7)
OW	0.0927 (6)	0.8909 (4)	0.6132 (4)	0.165 (3)
H1W	0.1292	0.9532	0.6108	0.198*
H2W	0.0289	0.8885	0.5880	0.198*
N1	0.3242 (2)	0.49721 (19)	0.6666 (2)	0.0248 (6)
N2	0.1075 (3)	0.3999 (2)	0.6983 (2)	0.0336 (8)
N3	0.0507 (3)	0.5696 (2)	0.6534 (2)	0.0360 (8)
N4	0.2758 (3)	0.4229 (2)	0.1511 (2)	0.0386 (8)
N5	0.2740 (3)	0.6711 (2)	0.7577 (2)	0.0322 (8)
N6	0.3669 (3)	0.2700 (2)	0.0528 (2)	0.0395 (8)
N7	0.0811 (3)	0.2755 (2)	0.0120 (2)	0.0381 (8)
N8	0.1195 (3)	0.1703 (2)	0.1429 (2)	0.0363 (8)
C1	0.5395 (3)	0.3730 (3)	0.0581 (3)	0.0402 (10)
C2	0.4044 (3)	0.5759 (2)	0.6806 (2)	0.0252 (8)
C3	−0.0922 (4)	0.1766 (3)	−0.0322 (3)	0.0433 (10)
C4	0.0147 (3)	0.3924 (3)	0.6471 (3)	0.0342 (9)
C5	0.3761 (3)	0.6697 (2)	0.7290 (2)	0.0268 (8)
C6	0.4517 (3)	0.7547 (3)	0.7449 (3)	0.0311 (9)
C7	0.4304 (3)	0.3587 (3)	0.0796 (3)	0.0328 (9)
C8	−0.1153 (4)	0.4805 (4)	0.5745 (3)	0.0467 (11)
C9	0.3806 (3)	0.4410 (3)	0.1307 (3)	0.0325 (9)
C10	0.2811 (5)	0.5963 (3)	0.2206 (3)	0.0585 (14)
H10	0.2445	0.6482	0.2509	0.070*
C11	0.3486 (3)	0.4095 (2)	0.6197 (3)	0.0320 (9)
H11	0.2947	0.3553	0.6077	0.038*
C12	−0.0767 (4)	0.6581 (4)	0.5864 (3)	0.0593 (15)
H12	−0.0957	0.7192	0.5755	0.071*
C13	0.5502 (4)	0.5474 (3)	0.1329 (3)	0.0499 (12)
H13	0.5898	0.6104	0.1497	0.060*
C14	0.4405 (4)	0.5360 (3)	0.1564 (3)	0.0408 (10)
C15	0.3139 (4)	0.8467 (3)	0.8150 (3)	0.0557 (14)
H15	0.2895	0.9071	0.8428	0.067*
C16	−0.0132 (4)	0.2146 (3)	0.6412 (4)	0.0569 (14)
H16	−0.0531	0.1521	0.6219	0.068*
C17	−0.0180 (3)	0.4838 (3)	0.6247 (3)	0.0355 (9)
C18	0.0585 (4)	0.3337 (3)	−0.0460 (3)	0.0521 (12)
H18	0.1092	0.3875	−0.0508	0.062*
C19	0.0269 (3)	0.1424 (3)	0.0902 (3)	0.0326 (9)
C20	0.1382 (4)	0.3162 (3)	0.7199 (3)	0.0415 (11)
H20	0.2014	0.3209	0.7559	0.050*
C21	−0.0245 (4)	0.0114 (3)	0.1713 (4)	0.0543 (13)
H21	−0.0721	−0.0423	0.1814	0.065*
C22	−0.1800 (4)	0.3849 (4)	0.5459 (3)	0.0597 (14)
H22	−0.2453	0.3819	0.5131	0.072*
C23	0.0041 (3)	0.1999 (3)	0.0214 (3)	0.0329 (9)
C24	−0.1094 (4)	0.2405 (4)	−0.0941 (3)	0.0562 (13)

H24	−0.1722	0.2285	−0.1316	0.067*
C25	0.4181 (4)	0.8454 (3)	0.7888 (3)	0.0454 (12)
H25	0.4657	0.9041	0.8000	0.054*
C26	0.5586 (3)	0.7450 (3)	0.7127 (3)	0.0417 (10)
H26	0.6097	0.8013	0.7230	0.050*
C27	−0.1482 (4)	0.3006 (4)	0.5655 (3)	0.0621 (15)
H27	−0.1907	0.2397	0.5444	0.075*
C28	0.0799 (4)	0.2219 (3)	0.6910 (4)	0.0522 (13)
H28	0.1051	0.1648	0.7059	0.063*
C29	0.5081 (3)	0.5680 (3)	0.6501 (3)	0.0343 (9)
C30	−0.0352 (5)	0.3193 (4)	−0.0994 (3)	0.0611 (14)
H30	−0.0478	0.3628	−0.1386	0.073*
C31	0.4503 (4)	0.3952 (3)	0.5881 (3)	0.0459 (12)
H31	0.4644	0.3320	0.5571	0.055*
C32	0.0673 (4)	0.0393 (3)	0.2246 (4)	0.0558 (13)
H32	0.0830	0.0055	0.2712	0.067*
C33	−0.1430 (4)	0.5724 (5)	0.5569 (3)	0.0626 (15)
H33	−0.2074	0.5743	0.5245	0.075*
C34	−0.0503 (4)	0.3012 (3)	0.6183 (3)	0.0454 (11)
C35	0.5864 (3)	0.6571 (3)	0.6685 (3)	0.0445 (11)
H35	0.6565	0.6527	0.6492	0.053*
C36	0.5200 (5)	0.2028 (4)	−0.0215 (4)	0.0658 (15)
H36	0.5478	0.1482	−0.0571	0.079*
C37	0.5992 (4)	0.4702 (4)	0.0870 (3)	0.0522 (13)
H37	0.6717	0.4802	0.0741	0.063*
C38	0.0218 (4)	0.6541 (3)	0.6342 (3)	0.0484 (12)
H38	0.0680	0.7132	0.6527	0.058*
C39	0.1380 (4)	0.1196 (3)	0.2086 (3)	0.0460 (11)
H39	0.2010	0.1386	0.2456	0.055*
C40	0.3853 (5)	0.6149 (3)	0.2028 (3)	0.0539 (13)
H40	0.4211	0.6795	0.2209	0.065*
C41	0.5838 (4)	0.2910 (4)	0.0069 (3)	0.0550 (13)
H41	0.6561	0.2968	−0.0076	0.066*
C42	−0.0492 (3)	0.0616 (3)	0.1013 (3)	0.0407 (10)
C43	0.2444 (4)	0.7583 (3)	0.8004 (3)	0.0494 (12)
H43	0.1747	0.7601	0.8212	0.059*
C44	0.5293 (4)	0.4732 (3)	0.6022 (3)	0.0478 (12)
H44	0.5975	0.4641	0.5802	0.057*
C45	−0.1650 (4)	0.0919 (4)	−0.0218 (3)	0.0529 (12)
H45	−0.2280	0.0746	−0.0588	0.063*
C46	0.2274 (4)	0.5000 (3)	0.1941 (3)	0.0542 (13)
H46	0.1549	0.4890	0.2068	0.065*
C47	−0.1435 (4)	0.0372 (3)	0.0408 (4)	0.0525 (13)
H47	−0.1915	−0.0186	0.0452	0.063*
C48	0.4124 (4)	0.1944 (3)	0.0030 (3)	0.0561 (13)
H48	0.3704	0.1330	−0.0165	0.067*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.02267 (17)	0.01487 (13)	0.02523 (17)	−0.00025 (11)	−0.00352 (13)	0.00268 (12)
Mo2	0.02224 (18)	0.02282 (15)	0.02934 (18)	0.00244 (12)	−0.00481 (14)	0.00147 (13)
Mo3	0.02799 (19)	0.02052 (15)	0.03045 (18)	0.00442 (12)	−0.00292 (14)	0.00071 (13)
Mo4	0.02487 (18)	0.02240 (15)	0.02754 (18)	0.00159 (12)	−0.00516 (14)	0.00228 (13)
Cu1	0.0234 (3)	0.0210 (2)	0.0403 (3)	−0.00076 (17)	0.0026 (2)	0.00364 (19)
Cu2	0.0349 (3)	0.0446 (3)	0.0647 (4)	−0.0091 (2)	−0.0045 (3)	0.0101 (3)
Cl	0.0579 (8)	0.0440 (5)	0.0462 (7)	0.0020 (5)	0.0203 (6)	0.0074 (5)
O1	0.0411 (18)	0.0226 (12)	0.0440 (17)	−0.0079 (11)	−0.0104 (14)	0.0091 (12)
O2	0.0283 (15)	0.0196 (11)	0.0344 (15)	0.0022 (10)	−0.0070 (12)	−0.0036 (10)
O3	0.0306 (15)	0.0258 (12)	0.0265 (14)	0.0068 (10)	−0.0041 (11)	0.0045 (10)
O4	0.0275 (15)	0.0244 (12)	0.0277 (14)	0.0034 (10)	−0.0055 (11)	0.0060 (10)
O5	0.0496 (19)	0.0359 (14)	0.0289 (15)	0.0059 (13)	0.0032 (13)	0.0038 (12)
O6	0.0264 (15)	0.0298 (12)	0.0306 (15)	0.0023 (11)	−0.0051 (12)	−0.0022 (11)
O7	0.0272 (16)	0.0446 (15)	0.0515 (19)	−0.0059 (12)	−0.0045 (14)	0.0045 (14)
O8	0.0445 (19)	0.0272 (13)	0.0468 (18)	0.0123 (12)	−0.0096 (14)	0.0027 (12)
O9	0.0369 (16)	0.0223 (11)	0.0268 (14)	0.0074 (11)	−0.0029 (12)	0.0023 (10)
O10	0.0287 (15)	0.0292 (12)	0.0286 (14)	0.0003 (11)	0.0019 (12)	0.0031 (11)
O11	0.0388 (17)	0.0405 (14)	0.0347 (16)	0.0041 (12)	−0.0017 (13)	0.0101 (12)
O12	0.0381 (18)	0.0266 (13)	0.0524 (19)	0.0079 (12)	−0.0054 (14)	−0.0019 (12)
O13	0.0331 (17)	0.0385 (14)	0.0398 (17)	−0.0067 (12)	−0.0082 (13)	0.0006 (12)
OW	0.213 (7)	0.127 (4)	0.152 (6)	−0.030 (4)	0.083 (5)	0.037 (4)
N1	0.0259 (17)	0.0219 (14)	0.0268 (17)	0.0028 (12)	0.0002 (13)	0.0054 (12)
N2	0.0262 (19)	0.0266 (15)	0.046 (2)	−0.0013 (13)	0.0060 (16)	0.0047 (15)
N3	0.031 (2)	0.0383 (17)	0.040 (2)	0.0071 (15)	0.0026 (16)	0.0089 (15)
N4	0.044 (2)	0.0366 (17)	0.033 (2)	0.0022 (16)	0.0020 (17)	0.0031 (15)
N5	0.033 (2)	0.0191 (14)	0.042 (2)	−0.0008 (13)	0.0083 (16)	0.0000 (13)
N6	0.037 (2)	0.0353 (17)	0.043 (2)	0.0013 (15)	−0.0011 (17)	0.0006 (15)
N7	0.037 (2)	0.0401 (18)	0.038 (2)	0.0047 (15)	0.0007 (16)	0.0075 (16)
N8	0.030 (2)	0.0353 (17)	0.044 (2)	0.0050 (14)	−0.0040 (16)	0.0077 (16)
C1	0.032 (2)	0.056 (2)	0.034 (2)	−0.0001 (19)	−0.0048 (19)	0.016 (2)
C2	0.024 (2)	0.0277 (17)	0.0243 (19)	0.0025 (15)	0.0012 (16)	0.0062 (15)
C3	0.036 (3)	0.054 (2)	0.034 (2)	0.015 (2)	−0.003 (2)	−0.011 (2)
C4	0.025 (2)	0.038 (2)	0.035 (2)	−0.0075 (16)	0.0064 (18)	0.0011 (17)
C5	0.027 (2)	0.0281 (17)	0.026 (2)	−0.0007 (15)	0.0005 (16)	0.0085 (15)
C6	0.036 (2)	0.0279 (18)	0.029 (2)	−0.0078 (16)	−0.0032 (18)	0.0108 (16)
C7	0.031 (2)	0.036 (2)	0.028 (2)	−0.0037 (17)	−0.0052 (18)	0.0059 (17)
C8	0.026 (2)	0.081 (3)	0.032 (2)	0.013 (2)	0.006 (2)	0.007 (2)
C9	0.038 (2)	0.0321 (19)	0.026 (2)	0.0010 (17)	−0.0038 (18)	0.0062 (16)
C10	0.091 (5)	0.037 (2)	0.048 (3)	0.021 (3)	0.007 (3)	0.001 (2)
C11	0.045 (3)	0.0215 (17)	0.029 (2)	0.0092 (16)	0.0017 (18)	0.0023 (15)
C12	0.061 (4)	0.079 (4)	0.052 (3)	0.041 (3)	0.013 (3)	0.030 (3)
C13	0.057 (3)	0.040 (2)	0.049 (3)	−0.018 (2)	−0.018 (2)	0.016 (2)
C14	0.053 (3)	0.036 (2)	0.031 (2)	−0.0075 (19)	−0.008 (2)	0.0090 (18)
C15	0.066 (4)	0.026 (2)	0.069 (3)	−0.005 (2)	0.025 (3)	−0.005 (2)

C16	0.062 (4)	0.032 (2)	0.066 (3)	−0.020 (2)	0.029 (3)	−0.009 (2)
C17	0.025 (2)	0.050 (2)	0.030 (2)	0.0003 (18)	0.0040 (18)	0.0051 (18)
C18	0.058 (3)	0.054 (3)	0.047 (3)	0.007 (2)	0.006 (3)	0.018 (2)
C19	0.025 (2)	0.0356 (19)	0.037 (2)	0.0085 (16)	0.0054 (18)	0.0047 (17)
C20	0.037 (3)	0.033 (2)	0.057 (3)	0.0056 (18)	0.010 (2)	0.014 (2)
C21	0.053 (3)	0.040 (2)	0.074 (4)	0.004 (2)	0.022 (3)	0.020 (2)
C22	0.023 (3)	0.106 (4)	0.039 (3)	−0.012 (3)	−0.002 (2)	−0.002 (3)
C23	0.029 (2)	0.036 (2)	0.032 (2)	0.0106 (17)	0.0017 (18)	−0.0024 (17)
C24	0.047 (3)	0.086 (4)	0.032 (3)	0.027 (3)	−0.009 (2)	−0.005 (2)
C25	0.063 (3)	0.0262 (19)	0.042 (3)	−0.0152 (19)	0.007 (2)	0.0037 (18)
C26	0.032 (2)	0.041 (2)	0.053 (3)	−0.0110 (18)	−0.007 (2)	0.020 (2)
C27	0.042 (3)	0.078 (3)	0.050 (3)	−0.028 (3)	0.009 (3)	−0.013 (3)
C28	0.062 (4)	0.028 (2)	0.069 (3)	−0.001 (2)	0.031 (3)	0.013 (2)
C29	0.031 (2)	0.037 (2)	0.040 (2)	0.0072 (17)	0.0056 (19)	0.0187 (19)
C30	0.075 (4)	0.080 (4)	0.034 (3)	0.025 (3)	0.001 (3)	0.017 (3)
C31	0.064 (3)	0.030 (2)	0.048 (3)	0.020 (2)	0.021 (2)	0.0067 (19)
C32	0.057 (3)	0.055 (3)	0.064 (3)	0.010 (2)	0.009 (3)	0.029 (3)
C33	0.040 (3)	0.112 (4)	0.040 (3)	0.028 (3)	−0.001 (2)	0.015 (3)
C34	0.036 (3)	0.051 (3)	0.039 (3)	−0.015 (2)	0.011 (2)	−0.007 (2)
C35	0.020 (2)	0.052 (3)	0.066 (3)	−0.0026 (18)	0.009 (2)	0.026 (2)
C36	0.069 (4)	0.061 (3)	0.066 (4)	0.025 (3)	0.013 (3)	−0.001 (3)
C37	0.033 (3)	0.071 (3)	0.054 (3)	−0.016 (2)	−0.012 (2)	0.030 (3)
C38	0.053 (3)	0.050 (3)	0.048 (3)	0.020 (2)	0.010 (2)	0.015 (2)
C39	0.038 (3)	0.054 (3)	0.049 (3)	0.010 (2)	−0.009 (2)	0.015 (2)
C40	0.089 (4)	0.029 (2)	0.039 (3)	0.001 (2)	−0.011 (3)	−0.0011 (19)
C41	0.039 (3)	0.081 (3)	0.051 (3)	0.016 (3)	0.011 (2)	0.021 (3)
C42	0.032 (2)	0.033 (2)	0.054 (3)	0.0048 (18)	0.011 (2)	0.0014 (19)
C43	0.052 (3)	0.0266 (19)	0.068 (3)	0.0042 (19)	0.028 (3)	0.003 (2)
C44	0.045 (3)	0.048 (2)	0.061 (3)	0.027 (2)	0.027 (2)	0.025 (2)
C45	0.034 (3)	0.067 (3)	0.046 (3)	0.009 (2)	−0.005 (2)	−0.017 (2)
C46	0.064 (4)	0.049 (3)	0.051 (3)	0.019 (2)	0.014 (3)	0.006 (2)
C47	0.030 (3)	0.046 (2)	0.070 (4)	−0.004 (2)	0.011 (2)	−0.014 (2)
C48	0.054 (3)	0.046 (3)	0.059 (3)	0.004 (2)	0.004 (3)	−0.011 (2)

Geometric parameters (Å, °)

Mo1—O1	1.701 (2)	C8—C33	1.399 (7)
Mo1—O9^{i}	1.784 (2)	C8—C22	1.441 (7)
Mo1—O6	1.786 (3)	C9—C14	1.403 (5)
Mo1—O3	1.790 (2)	C10—C40	1.338 (7)
Mo2—O7	1.693 (3)	C10—C46	1.388 (6)
Mo2—O8	1.695 (2)	C10—H10	0.9300
Mo2—O4	1.908 (2)	C11—C31	1.382 (6)
Mo2—O10^{i}	1.924 (2)	C11—H11	0.9300
Mo2—O6^{i}	2.354 (3)	C12—C33	1.349 (7)
Mo2—O3	2.424 (2)	C12—C38	1.411 (7)
Mo3—O12	1.692 (2)	C12—H12	0.9300
Mo3—O5	1.692 (3)	C13—C37	1.348 (7)

Mo3—O10	1.905 (3)	C13—C14	1.418 (6)
Mo3—O2	1.917 (3)	C13—H13	0.9300
Mo3—O9	2.380 (2)	C14—C40	1.411 (6)
Mo3—O6	2.499 (3)	C15—C25	1.364 (6)
Mo4—O13	1.694 (3)	C15—C43	1.385 (6)
Mo4—O11	1.703 (3)	C15—H15	0.9300
Mo4—O2	1.891 (2)	C16—C28	1.343 (7)
Mo4—O4	1.905 (2)	C16—C34	1.407 (7)
Mo4—O3	2.410 (2)	C16—H16	0.9300
Cu1—N5	1.984 (3)	C18—C30	1.369 (7)
Cu1—N2	1.992 (3)	C18—H18	0.9300
Cu1—N1	2.075 (3)	C19—C42	1.413 (5)
Cu1—N3	2.177 (3)	C19—C23	1.443 (5)
Cu1—Cl	2.2750 (12)	C20—C28	1.391 (6)
Cu2—N8	2.025 (3)	C20—H20	0.9300
Cu2—N4	2.028 (3)	C21—C32	1.352 (7)
Cu2—N6	2.044 (4)	C21—C42	1.397 (6)
Cu2—N7	2.047 (4)	C21—H21	0.9300
O6—Mo2^{i}	2.354 (3)	C22—C27	1.332 (7)
O9—Mo1^{i}	1.784 (2)	C22—H22	0.9300
O10—Mo2^{i}	1.924 (2)	C24—C30	1.358 (7)
OW—H1W	0.9273	C24—H24	0.9300
OW—H2W	0.8637	C25—H25	0.9300
N1—C11	1.329 (4)	C26—C35	1.333 (6)
N1—C2	1.367 (4)	C26—H26	0.9300
N2—C20	1.331 (5)	C27—C34	1.430 (7)
N2—C4	1.351 (5)	C27—H27	0.9300
N3—C38	1.318 (5)	C28—H28	0.9300
N3—C17	1.364 (5)	C29—C44	1.403 (6)
N4—C46	1.328 (5)	C29—C35	1.451 (5)
N4—C9	1.355 (5)	C30—H30	0.9300
N5—C43	1.326 (5)	C31—C44	1.351 (6)
N5—C5	1.352 (5)	C31—H31	0.9300
N6—C48	1.333 (5)	C32—C39	1.392 (6)
N6—C7	1.357 (5)	C32—H32	0.9300
N7—C18	1.323 (5)	C33—H33	0.9300
N7—C23	1.362 (5)	C35—H35	0.9300
N8—C39	1.330 (5)	C36—C41	1.356 (7)
N8—C19	1.356 (5)	C36—C48	1.396 (7)
C1—C41	1.397 (6)	C36—H36	0.9300
C1—C7	1.405 (6)	C37—H37	0.9300
C1—C37	1.431 (6)	C38—H38	0.9300
C2—C29	1.387 (5)	C39—H39	0.9300
C2—C5	1.422 (5)	C40—H40	0.9300
C3—C23	1.396 (6)	C41—H41	0.9300
C3—C24	1.409 (6)	C42—C47	1.430 (6)
C3—C45	1.426 (6)	C43—H43	0.9300
C4—C34	1.396 (5)	C44—H44	0.9300

C4—C17	1.443 (5)	C45—C47	1.339 (7)
C5—C6	1.392 (5)	C45—H45	0.9300
C6—C25	1.391 (5)	C46—H46	0.9300
C6—C26	1.435 (6)	C47—H47	0.9300
C7—C9	1.434 (5)	C48—H48	0.9300
C8—C17	1.398 (6)		
O1—Mo1—O9^{i}	110.77 (12)	N4—C9—C14	122.9 (4)
O1—Mo1—O6	108.63 (12)	N4—C9—C7	117.6 (3)
O9^{i}—Mo1—O6	108.98 (12)	C14—C9—C7	119.6 (4)
O1—Mo1—O3	109.46 (12)	C40—C10—C46	120.4 (4)
O9^{i}—Mo1—O3	109.75 (11)	C40—C10—H10	119.8
O6—Mo1—O3	109.22 (11)	C46—C10—H10	119.8
O7—Mo2—O8	104.51 (14)	N1—C11—C31	122.9 (4)
O7—Mo2—O4	99.96 (13)	N1—C11—H11	118.6
O8—Mo2—O4	100.05 (12)	C31—C11—H11	118.6
O7—Mo2—O10^{i}	98.57 (12)	C33—C12—C38	119.3 (4)
O8—Mo2—O10^{i}	103.19 (12)	C33—C12—H12	120.3
O4—Mo2—O10^{i}	145.44 (10)	C38—C12—H12	120.3
O7—Mo2—O6^{i}	165.89 (11)	C37—C13—C14	122.5 (4)
O8—Mo2—O6^{i}	88.84 (11)	C37—C13—H13	118.8
O4—Mo2—O6^{i}	81.81 (10)	C14—C13—H13	118.8
O10^{i}—Mo2—O6^{i}	73.50 (10)	C9—C14—C40	116.7 (4)
O7—Mo2—O3	91.97 (11)	C9—C14—C13	118.8 (4)
O8—Mo2—O3	162.84 (11)	C40—C14—C13	124.5 (4)
O4—Mo2—O3	71.92 (8)	C25—C15—C43	120.1 (4)
O10^{i}—Mo2—O3	78.54 (9)	C25—C15—H15	119.9
O6^{i}—Mo2—O3	75.18 (8)	C43—C15—H15	119.9
O12—Mo3—O5	104.20 (13)	C28—C16—C34	120.1 (4)
O12—Mo3—O10	100.90 (12)	C28—C16—H16	119.9
O5—Mo3—O10	102.03 (12)	C34—C16—H16	119.9
O12—Mo3—O2	97.65 (12)	N3—C17—C8	123.7 (4)
O5—Mo3—O2	104.17 (13)	N3—C17—C4	116.7 (4)
O10—Mo3—O2	142.88 (11)	C8—C17—C4	119.6 (4)
O12—Mo3—O9	165.05 (11)	N7—C18—C30	123.7 (5)
O5—Mo3—O9	89.52 (10)	N7—C18—H18	118.1
O10—Mo3—O9	81.60 (9)	C30—C18—H18	118.1
O2—Mo3—O9	72.83 (9)	N8—C19—C42	123.0 (4)
O12—Mo3—O6	90.89 (11)	N8—C19—C23	118.2 (3)
O5—Mo3—O6	164.31 (10)	C42—C19—C23	118.8 (4)
O10—Mo3—O6	70.35 (9)	N2—C20—C28	122.9 (5)
O2—Mo3—O6	77.53 (10)	N2—C20—H20	118.6
O9—Mo3—O6	75.97 (8)	C28—C20—H20	118.6
O13—Mo4—O11	104.46 (13)	C32—C21—C42	121.2 (4)
O13—Mo4—O2	101.17 (12)	C32—C21—H21	119.4
O11—Mo4—O2	101.42 (12)	C42—C21—H21	119.4
O13—Mo4—O4	103.89 (12)	C27—C22—C8	121.3 (5)

O11—Mo4—O4	99.44 (11)	C27—C22—H22	119.3
O2—Mo4—O4	142.00 (10)	C8—C22—H22	119.3
O13—Mo4—O3	86.90 (11)	N7—C23—C3	123.2 (4)
O11—Mo4—O3	167.48 (11)	N7—C23—C19	116.5 (4)
O2—Mo4—O3	81.10 (9)	C3—C23—C19	120.3 (4)
O4—Mo4—O3	72.28 (8)	C30—C24—C3	120.6 (5)
N5—Cu1—N2	174.07 (13)	C30—C24—H24	119.7
N5—Cu1—N1	80.90 (12)	C3—C24—H24	119.7
N2—Cu1—N1	93.84 (12)	C15—C25—C6	118.9 (4)
N5—Cu1—N3	100.17 (13)	C15—C25—H25	120.6
N2—Cu1—N3	79.86 (13)	C6—C25—H25	120.6
N1—Cu1—N3	118.23 (12)	C35—C26—C6	121.6 (4)
N5—Cu1—Cl	93.57 (10)	C35—C26—H26	119.2
N2—Cu1—Cl	92.28 (10)	C6—C26—H26	119.2
N1—Cu1—Cl	142.65 (9)	C22—C27—C34	121.7 (5)
N3—Cu1—Cl	99.12 (10)	C22—C27—H27	119.2
N8—Cu2—N4	135.47 (14)	C34—C27—H27	119.2
N8—Cu2—N6	126.33 (13)	C16—C28—C20	119.1 (4)
N4—Cu2—N6	82.10 (13)	C16—C28—H28	120.4
N8—Cu2—N7	82.78 (13)	C20—C28—H28	120.4
N4—Cu2—N7	111.32 (13)	C2—C29—C44	116.8 (4)
N6—Cu2—N7	123.38 (14)	C2—C29—C35	118.7 (4)
Mo4—O2—Mo3	125.75 (12)	C44—C29—C35	124.5 (4)
Mo1—O3—Mo4	130.38 (12)	C24—C30—C18	118.9 (5)
Mo1—O3—Mo2	131.05 (12)	C24—C30—H30	120.5
Mo4—O3—Mo2	88.10 (7)	C18—C30—H30	120.5
Mo4—O4—Mo2	123.63 (11)	C44—C31—C11	119.9 (4)
Mo1—O6—Mo2^{i}	132.46 (13)	C44—C31—H31	120.1
Mo1—O6—Mo3	130.64 (12)	C11—C31—H31	120.1
Mo2^{i}—O6—Mo3	88.22 (8)	C21—C32—C39	118.9 (4)
Mo1^{i}—O9—Mo3	129.93 (12)	C21—C32—H32	120.6
Mo3—O10—Mo2^{i}	123.90 (12)	C39—C32—H32	120.6
H1W—OW—H2W	107.4	C12—C33—C8	120.4 (5)
C11—N1—C2	117.0 (3)	C12—C33—H33	119.8
C11—N1—Cu1	131.6 (3)	C8—C33—H33	119.8
C2—N1—Cu1	111.2 (2)	C4—C34—C16	117.2 (4)
C20—N2—C4	118.0 (3)	C4—C34—C27	118.7 (4)
C20—N2—Cu1	125.9 (3)	C16—C34—C27	124.0 (4)
C4—N2—Cu1	116.1 (2)	C26—C35—C29	120.6 (4)
C38—N3—C17	117.6 (4)	C26—C35—H35	119.7
C38—N3—Cu1	132.4 (3)	C29—C35—H35	119.7
C17—N3—Cu1	109.8 (2)	C41—C36—C48	119.8 (5)
C46—N4—C9	118.0 (4)	C41—C36—H36	120.1
C46—N4—Cu2	129.9 (3)	C48—C36—H36	120.1
C9—N4—Cu2	111.8 (2)	C13—C37—C1	120.0 (4)
C43—N5—C5	118.0 (3)	C13—C37—H37	120.0
C43—N5—Cu1	127.5 (3)	C1—C37—H37	120.0
C5—N5—Cu1	114.5 (2)	N3—C38—C12	122.4 (5)

C48—N6—C7	116.8 (4)	N3—C38—H38	118.8
C48—N6—Cu2	131.6 (3)	C12—C38—H38	118.8
C7—N6—Cu2	111.6 (3)	N8—C39—C32	122.9 (4)
C18—N7—C23	117.4 (4)	N8—C39—H39	118.5
C18—N7—Cu2	131.5 (3)	C32—C39—H39	118.5
C23—N7—Cu2	111.0 (3)	C10—C40—C14	119.7 (4)
C39—N8—C19	117.9 (3)	C10—C40—H40	120.2
C39—N8—Cu2	130.9 (3)	C14—C40—H40	120.2
C19—N8—Cu2	110.9 (2)	C36—C41—C1	119.2 (5)
C41—C1—C7	117.6 (4)	C36—C41—H41	120.4
C41—C1—C37	123.0 (4)	C1—C41—H41	120.4
C7—C1—C37	119.3 (4)	C21—C42—C19	116.1 (4)
N1—C2—C29	123.6 (3)	C21—C42—C47	125.4 (4)
N1—C2—C5	116.1 (3)	C19—C42—C47	118.5 (4)
C29—C2—C5	120.2 (3)	N5—C43—C15	122.2 (4)
C23—C3—C24	115.9 (4)	N5—C43—H43	118.9
C23—C3—C45	119.2 (4)	C15—C43—H43	118.9
C24—C3—C45	124.8 (4)	C31—C44—C29	119.8 (4)
N2—C4—C34	122.5 (4)	C31—C44—H44	120.1
N2—C4—C17	117.4 (3)	C29—C44—H44	120.1
C34—C4—C17	120.0 (4)	C47—C45—C3	120.7 (4)
N5—C5—C6	122.9 (3)	C47—C45—H45	119.7
N5—C5—C2	116.8 (3)	C3—C45—H45	119.7
C6—C5—C2	120.3 (3)	N4—C46—C10	122.3 (5)
C25—C6—C5	117.8 (4)	N4—C46—H46	118.8
C25—C6—C26	123.6 (4)	C10—C46—H46	118.8
C5—C6—C26	118.6 (3)	C45—C47—C42	122.2 (4)
N6—C7—C1	123.3 (4)	C45—C47—H47	118.9
N6—C7—C9	116.8 (4)	C42—C47—H47	118.9
C1—C7—C9	119.8 (4)	N6—C48—C36	123.3 (5)
C17—C8—C33	116.5 (5)	N6—C48—H48	118.4
C17—C8—C22	118.6 (4)	C36—C48—H48	118.4
C33—C8—C22	124.9 (5)		
O13—Mo4—O2—Mo3	−176.59 (16)	N1—C2—C5—C6	−178.6 (3)
O11—Mo4—O2—Mo3	−69.16 (18)	C29—C2—C5—C6	1.1 (5)
O4—Mo4—O2—Mo3	52.9 (3)	N5—C5—C6—C25	−2.9 (6)
O3—Mo4—O2—Mo3	98.39 (16)	C2—C5—C6—C25	177.0 (3)
O12—Mo3—O2—Mo4	171.57 (17)	N5—C5—C6—C26	179.1 (3)
O5—Mo3—O2—Mo4	64.75 (18)	C2—C5—C6—C26	−1.0 (5)
O10—Mo3—O2—Mo4	−68.9 (2)	C48—N6—C7—C1	−0.6 (6)
O9—Mo3—O2—Mo4	−20.25 (14)	Cu2—N6—C7—C1	179.9 (3)
O6—Mo3—O2—Mo4	−99.21 (16)	C48—N6—C7—C9	178.0 (4)
O1—Mo1—O3—Mo4	107.35 (17)	Cu2—N6—C7—C9	−1.4 (4)
$O9^{i}$—Mo1—O3—Mo4	−130.89 (15)	C41—C1—C7—N6	−0.3 (6)
O6—Mo1—O3—Mo4	−11.47 (18)	C37—C1—C7—N6	178.0 (4)
O1—Mo1—O3—Mo2	−119.58 (16)	C41—C1—C7—C9	−178.9 (4)
$O9^{i}$—Mo1—O3—Mo2	2.18 (19)	C37—C1—C7—C9	−0.6 (6)
O6—Mo1—O3—Mo2	121.60 (15)	C46—N4—C9—C14	2.8 (6)

O13—Mo4—O3—Mo1	−120.29 (17)	Cu2—N4—C9—C14	177.1 (3)
O11—Mo4—O3—Mo1	84.2 (5)	C46—N4—C9—C7	−176.4 (4)
O2—Mo4—O3—Mo1	−18.47 (16)	Cu2—N4—C9—C7	−2.2 (4)
O4—Mo4—O3—Mo1	134.07 (18)	N6—C7—C9—N4	2.5 (5)
O13—Mo4—O3—Mo2	93.16 (11)	C1—C7—C9—N4	−178.8 (3)
O11—Mo4—O3—Mo2	−62.3 (5)	N6—C7—C9—C14	−176.8 (3)
O2—Mo4—O3—Mo2	−165.02 (10)	C1—C7—C9—C14	1.9 (5)
O4—Mo4—O3—Mo2	−12.48 (9)	C2—N1—C11—C31	1.9 (5)
O7—Mo2—O3—Mo1	126.49 (18)	Cu1—N1—C11—C31	−172.5 (3)
O8—Mo2—O3—Mo1	−69.5 (4)	N4—C9—C14—C40	−2.1 (6)
O4—Mo2—O3—Mo1	−133.67 (18)	C7—C9—C14—C40	177.1 (4)
O10^{i}—Mo2—O3—Mo1	28.14 (16)	N4—C9—C14—C13	179.3 (4)
O6^{i}—Mo2—O3—Mo1	−47.60 (16)	C7—C9—C14—C13	−1.5 (6)
O7—Mo2—O3—Mo4	−87.34 (12)	C37—C13—C14—C9	−0.2 (6)
O8—Mo2—O3—Mo4	76.7 (4)	C37—C13—C14—C40	−178.8 (4)
O4—Mo2—O3—Mo4	12.49 (9)	C38—N3—C17—C8	1.5 (6)
O10^{i}—Mo2—O3—Mo4	174.31 (10)	Cu1—N3—C17—C8	177.4 (3)
O6^{i}—Mo2—O3—Mo4	98.56 (9)	C38—N3—C17—C4	−179.5 (3)
O13—Mo4—O4—Mo2	−62.85 (17)	Cu1—N3—C17—C4	−3.6 (4)
O11—Mo4—O4—Mo2	−170.42 (16)	C33—C8—C17—N3	−2.3 (6)
O2—Mo4—O4—Mo2	67.0 (2)	C22—C8—C17—N3	178.5 (4)
O3—Mo4—O4—Mo2	19.25 (13)	C33—C8—C17—C4	178.7 (4)
O7—Mo2—O4—Mo4	69.65 (17)	C22—C8—C17—C4	−0.5 (6)
O8—Mo2—O4—Mo4	176.47 (16)	N2—C4—C17—N3	3.1 (5)
O10^{i}—Mo2—O4—Mo4	−51.8 (3)	C34—C4—C17—N3	−178.6 (4)
O6^{i}—Mo2—O4—Mo4	−96.18 (15)	N2—C4—C17—C8	−177.8 (4)
O3—Mo2—O4—Mo4	−19.18 (13)	C34—C4—C17—C8	0.4 (6)
O1—Mo1—O6—Mo2^{i}	111.78 (16)	C23—N7—C18—C30	−2.9 (7)
O9^{i}—Mo1—O6—Mo2^{i}	−8.99 (18)	Cu2—N7—C18—C30	179.2 (4)
O3—Mo1—O6—Mo2^{i}	−128.88 (15)	C39—N8—C19—C42	−0.9 (6)
O1—Mo1—O6—Mo3	−111.36 (16)	Cu2—N8—C19—C42	174.2 (3)
O9^{i}—Mo1—O6—Mo3	127.87 (14)	C39—N8—C19—C23	177.4 (4)
O3—Mo1—O6—Mo3	7.98 (18)	Cu2—N8—C19—C23	−7.5 (4)
O12—Mo3—O6—Mo1	121.68 (17)	C4—N2—C20—C28	1.0 (6)
O5—Mo3—O6—Mo1	−74.0 (5)	Cu1—N2—C20—C28	−178.6 (3)
O10—Mo3—O6—Mo1	−137.05 (17)	C17—C8—C22—C27	−0.7 (7)
O2—Mo3—O6—Mo1	24.05 (15)	C33—C8—C22—C27	−179.8 (5)
O9—Mo3—O6—Mo1	−51.10 (15)	C18—N7—C23—C3	5.3 (6)
O12—Mo3—O6—Mo2^{i}	−88.63 (11)	Cu2—N7—C23—C3	−176.4 (3)
O5—Mo3—O6—Mo2^{i}	75.7 (4)	C18—N7—C23—C19	−175.2 (4)
O10—Mo3—O6—Mo2^{i}	12.63 (8)	Cu2—N7—C23—C19	3.0 (4)
O2—Mo3—O6—Mo2^{i}	173.73 (9)	C24—C3—C23—N7	−3.9 (6)
O9—Mo3—O6—Mo2^{i}	98.59 (9)	C45—C3—C23—N7	175.9 (4)
O12—Mo3—O9—Mo1^{i}	−77.2 (5)	C24—C3—C23—C19	176.7 (4)
O5—Mo3—O9—Mo1^{i}	125.84 (18)	C45—C3—C23—C19	−3.5 (6)

O10—Mo3—O9—Mo1^{i}	23.61 (16)	N8—C19—C23—N7	3.0 (5)
O2—Mo3—O9—Mo1^{i}	−129.16 (18)	C42—C19—C23—N7	−178.6 (3)
O6—Mo3—O9—Mo1^{i}	−48.12 (15)	N8—C19—C23—C3	−177.5 (4)
O12—Mo3—O10—Mo2^{i}	68.23 (17)	C42—C19—C23—C3	0.8 (6)
O5—Mo3—O10—Mo2^{i}	175.48 (15)	C23—C3—C24—C30	−0.1 (7)
O2—Mo3—O10—Mo2^{i}	−50.4 (2)	C45—C3—C24—C30	−179.8 (5)
O9—Mo3—O10—Mo2^{i}	−96.82 (15)	C43—C15—C25—C6	1.9 (7)
O6—Mo3—O10—Mo2^{i}	−18.79 (12)	C5—C6—C25—C15	0.8 (6)
N5—Cu1—N1—C11	−179.1 (3)	C26—C6—C25—C15	178.7 (4)
N2—Cu1—N1—C11	−1.8 (3)	C25—C6—C26—C35	−177.9 (4)
N3—Cu1—N1—C11	−82.4 (3)	C5—C6—C26—C35	0.0 (6)
Cl—Cu1—N1—C11	97.0 (3)	C8—C22—C27—C34	2.0 (7)
N5—Cu1—N1—C2	6.3 (2)	C34—C16—C28—C20	0.5 (7)
N2—Cu1—N1—C2	−176.5 (2)	N2—C20—C28—C16	−2.0 (7)
N3—Cu1—N1—C2	103.0 (2)	N1—C2—C29—C44	0.3 (5)
Cl—Cu1—N1—C2	−77.6 (2)	C5—C2—C29—C44	−179.4 (4)
N1—Cu1—N2—C20	60.7 (3)	N1—C2—C29—C35	179.6 (3)
N3—Cu1—N2—C20	178.7 (3)	C5—C2—C29—C35	−0.1 (5)
Cl—Cu1—N2—C20	−82.5 (3)	C3—C24—C30—C18	2.3 (8)
N1—Cu1—N2—C4	−118.9 (3)	N7—C18—C30—C24	−0.8 (8)
N3—Cu1—N2—C4	−0.9 (3)	N1—C11—C31—C44	−1.9 (6)
Cl—Cu1—N2—C4	97.9 (3)	C42—C21—C32—C39	−0.2 (8)
N5—Cu1—N3—C38	−8.5 (4)	C38—C12—C33—C8	1.0 (7)
N2—Cu1—N3—C38	177.5 (4)	C17—C8—C33—C12	1.0 (7)
N1—Cu1—N3—C38	−93.5 (4)	C22—C8—C33—C12	−179.9 (4)
Cl—Cu1—N3—C38	86.8 (4)	N2—C4—C34—C16	−2.8 (6)
N5—Cu1—N3—C17	176.5 (3)	C17—C4—C34—C16	179.1 (4)
N2—Cu1—N3—C17	2.5 (3)	N2—C4—C34—C27	179.0 (4)
N1—Cu1—N3—C17	91.4 (3)	C17—C4—C34—C27	0.8 (6)
Cl—Cu1—N3—C17	−88.2 (3)	C28—C16—C34—C4	1.7 (7)
N8—Cu2—N4—C46	−50.1 (5)	C28—C16—C34—C27	179.9 (5)
N6—Cu2—N4—C46	174.5 (4)	C22—C27—C34—C4	−2.1 (7)
N7—Cu2—N4—C46	51.6 (4)	C22—C27—C34—C16	179.8 (4)
N8—Cu2—N4—C9	136.4 (3)	C6—C26—C35—C29	0.9 (6)
N6—Cu2—N4—C9	1.0 (3)	C2—C29—C35—C26	−0.9 (6)
N7—Cu2—N4—C9	−121.8 (3)	C44—C29—C35—C26	178.4 (4)
N1—Cu1—N5—C43	176.6 (4)	C14—C13—C37—C1	1.6 (7)
N3—Cu1—N5—C43	59.4 (4)	C41—C1—C37—C13	177.1 (4)
Cl—Cu1—N5—C43	−40.5 (4)	C7—C1—C37—C13	−1.2 (6)
N1—Cu1—N5—C5	−5.8 (3)	C17—N3—C38—C12	0.7 (6)
N3—Cu1—N5—C5	−123.0 (3)	Cu1—N3—C38—C12	−174.1 (3)
Cl—Cu1—N5—C5	137.0 (3)	C33—C12—C38—N3	−1.9 (7)
N8—Cu2—N6—C48	38.6 (5)	C19—N8—C39—C32	0.7 (7)
N4—Cu2—N6—C48	−179.1 (4)	Cu2—N8—C39—C32	−173.4 (4)
N7—Cu2—N6—C48	−68.8 (5)	C21—C32—C39—N8	−0.1 (8)
N8—Cu2—N6—C7	−142.1 (3)	C46—C10—C40—C14	0.3 (7)
N4—Cu2—N6—C7	0.2 (3)	C9—C14—C40—C10	0.5 (6)

N7—Cu2—N6—C7	110.6 (3)	C13—C14—C40—C10	179.1 (4)
N8—Cu2—N7—C18	172.5 (4)	C48—C36—C41—C1	−1.8 (8)
N4—Cu2—N7—C18	36.3 (4)	C7—C1—C41—C36	1.5 (7)
N6—Cu2—N7—C18	−58.3 (4)	C37—C1—C41—C36	−176.7 (4)
N8—Cu2—N7—C23	−5.4 (3)	C32—C21—C42—C19	−0.1 (7)
N4—Cu2—N7—C23	−141.7 (3)	C32—C21—C42—C47	179.3 (5)
N6—Cu2—N7—C23	123.7 (3)	N8—C19—C42—C21	0.6 (6)
N4—Cu2—N8—C39	−65.5 (4)	C23—C19—C42—C21	−177.6 (4)
N6—Cu2—N8—C39	54.8 (4)	N8—C19—C42—C47	−178.8 (4)
N7—Cu2—N8—C39	−178.7 (4)	C23—C19—C42—C47	2.9 (6)
N4—Cu2—N8—C19	120.1 (3)	C5—N5—C43—C15	0.8 (7)
N6—Cu2—N8—C19	−119.6 (3)	Cu1—N5—C43—C15	178.3 (4)
N7—Cu2—N8—C19	6.9 (3)	C25—C15—C43—N5	−2.8 (8)
C11—N1—C2—C29	−1.1 (5)	C11—C31—C44—C29	1.0 (7)
Cu1—N1—C2—C29	174.4 (3)	C2—C29—C44—C31	−0.2 (6)
C11—N1—C2—C5	178.6 (3)	C35—C29—C44—C31	−179.4 (4)
Cu1—N1—C2—C5	−5.9 (4)	C23—C3—C45—C47	2.3 (7)
C20—N2—C4—C34	1.4 (6)	C24—C3—C45—C47	−177.9 (4)
Cu1—N2—C4—C34	−178.9 (3)	C9—N4—C46—C10	−1.9 (7)
C20—N2—C4—C17	179.6 (3)	Cu2—N4—C46—C10	−175.0 (3)
Cu1—N2—C4—C17	−0.8 (5)	C40—C10—C46—N4	0.4 (8)
C43—N5—C5—C6	2.1 (6)	C3—C45—C47—C42	1.6 (7)
Cu1—N5—C5—C6	−175.7 (3)	C21—C42—C47—C45	176.4 (4)
C43—N5—C5—C2	−177.8 (4)	C19—C42—C47—C45	−4.2 (6)
Cu1—N5—C5—C2	4.4 (4)	C7—N6—C48—C36	0.3 (7)
N1—C2—C5—N5	1.3 (5)	Cu2—N6—C48—C36	179.6 (4)
C29—C2—C5—N5	−179.0 (3)	C41—C36—C48—N6	0.9 (8)

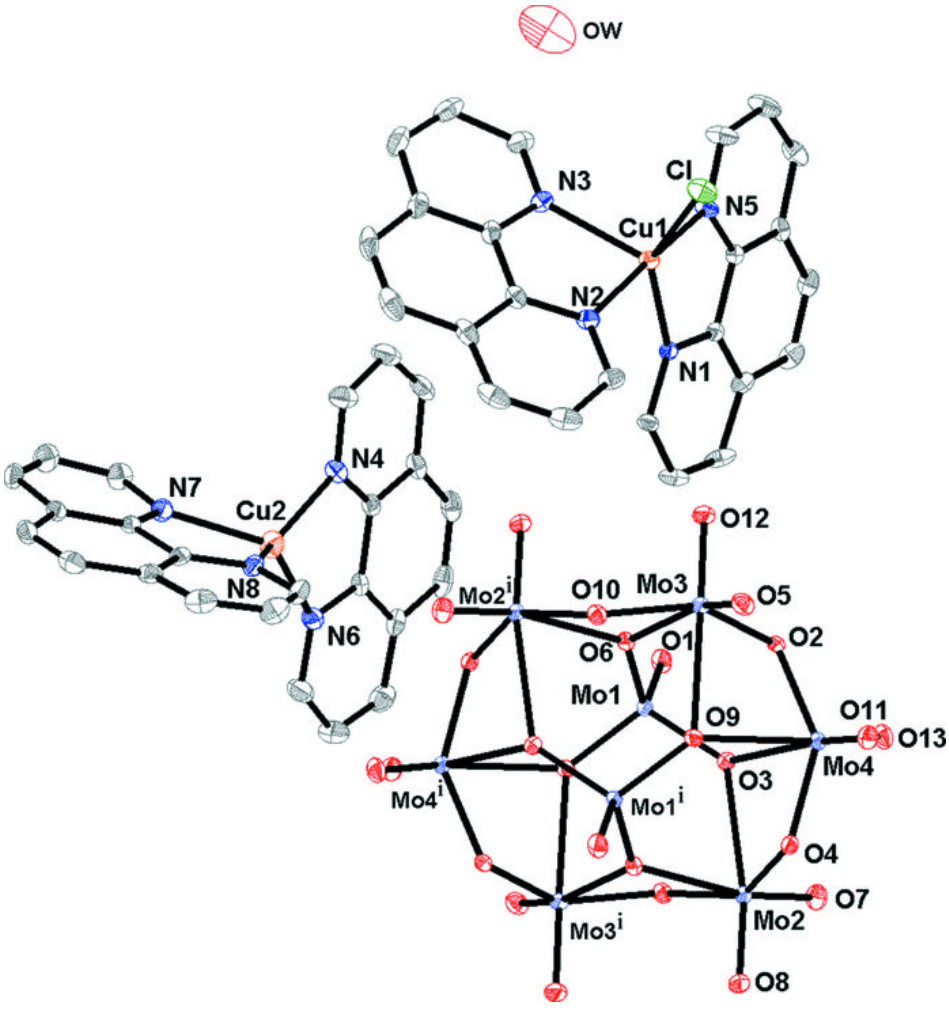
Symmetry codes: (i) −*x*+1, −*y*, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
OW—H1W···O7^{ii}	0.93	2.52	3.074 (6)	119
OW—H1W···O10^{iii}	0.93	2.15	3.005 (6)	152
C11—H11···O8^{i}	0.93	2.40	3.215 (5)	146
C12—H12···O8^{iv}	0.93	2.49	3.295 (5)	145
C16—H16···O7^{v}	0.93	2.41	3.320 (5)	166
C20—H20···O12	0.93	2.40	3.049 (5)	127
C22—H22···O1^{v}	0.93	2.53	3.213 (5)	131
C24—H24···O13^{vi}	0.93	2.41	3.164 (6)	138
C25—H25···O11^{iii}	0.93	2.41	3.301 (5)	161
C26—H26···O4^{iii}	0.93	2.58	3.327 (4)	137
C38—H38···OW	0.93	2.59	3.328 (6)	137
C40—H40···O2^{ii}	0.93	2.39	3.273 (5)	159

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

Fig. 1


OW
N3
Cl
N5
Cu1
N2
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Cu2
N8
N6
Mo2i
O10
Mo3
O12
O5
O6
O1
O2
Mo1
O9
O11
O13
Mo4
O3
Mo4i
Mo1i
O4
O7
Mo3i
Mo2
O8

Fig. 2