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# Bis{4,4′-[(2,2′-bi-1*H*-imidazole-1,1′-diyl)dimethylene]dipyridinium} *β*-octamolybdate

**Ya-Qian Lan, Jun-Sheng Qin and Zhong-Min Su***

Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China
Correspondence e-mail: ifmc9291@yahoo.com.cn

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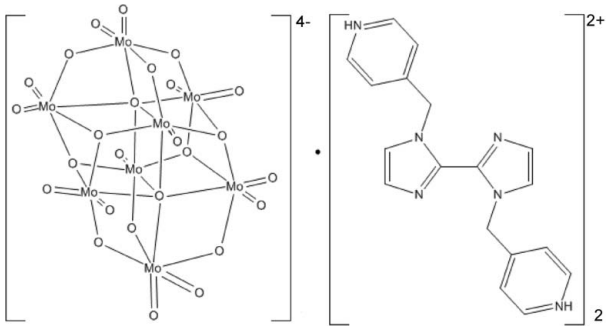
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.023; $wR$ factor = 0.054; data-to-parameter ratio = 16.2.

The title compound, $(C_{18}H_{18}N_6)_2[Mo_8O_{26}]$, was produced by hydrothermal reaction of an acidified aqueous solution of $Na_2MoO_4$ and 1,1′-bis(pyridin-4-ylmethyl)-2,2′-bi-1*H*-imidazole (hereafter *L*). The structure consists of the *β*-octamolybdate anions having a crystallographic center of symmetry and protonated $[H_2L]^{2+}$ cations. The $[H_2L]^{2+}$ cations link *β*-octamolybdate anions, generating a two-dimensional hydrogen-bonded supramolecular sheet.

## Related literature

For related literature on polyoxometalate (POM) chemistry, see: Pope (1983). Chen *et al.* (2002), Lu *et al.* (2002) and Reinoso *et al.* (2005) describe how the formation of metal complexes of polyoxometalates influences the POM frameworks and improves their electronic and magnetic properties.




## Experimental

### Crystal data

$(C_{18}H_{18}N_6)_2[Mo_8O_{26}]$
$M_r$ = 1820.28
Monoclinic, $C2/c$
$a$ = 23.1640 (4) Å
$b$ = 10.4740 (5) Å
$c$ = 22.7770 (8) Å
$\beta$ = 112.494 (1)°
$V$ = 5105.7 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 2.00 mm$^{-1}$
$T$ = 293 (2) K
0.28 × 0.26 × 0.19 mm

### Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.481, $T_{max}$ = 0.684
15475 measured reflections
6141 independent reflections
5242 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.020

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.054
$S$ = 1.01
6141 reflections
378 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.48 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N5—H5N···O11$^{i}$ | 0.79 (3) | 2.09 (3) | 2.801 (3) | 150 (3) |
| N6—H6N···O9$^{ii}$ | 0.79 (3) | 2.29 (4) | 2.923 (3) | 138 (3) |

Symmetry codes: (i) $-x+\frac{3}{2}, -y-\frac{1}{2}, -z$; (ii) $x, -y, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2074).

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# supplementary materials

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# Bis{4,4'-[(2,2'-bi-1*H*-imidazole-1,1'-diyl)dimethylene]dipyridinium} $\beta$-octamolybdate

**Y.-Q. Lan, J.-S. Qin and Z.-M. Su**

## Comment

Important advances in polyoxometalate (POM) chemistry (Pope, 1983) have recently been made in the coordination chemistry of polyoxoanions with classical transition metal coordination complexes or fragments. The introduction of metal complexes does not only enrich the frameworks of polyoxometalates but also ameliorates their electronic and magnetic properties (Chen *et al.*, 2002; Lu *et al.*, 2002; Reinoso *et al.*, 2005). During our ongoing studies of such materials, we obtained the title compound, and present its crystal structure here.

The asymmetric part of the unit cell contains each one $[H_2L]^{2+}$ cation and half a $[Mo_8O_{26}]^{4-}$ anion. The complete $[Mo_8O_{26}]^{4-}$ moiety is generated from the asymmetric unit atoms by a crystallographic inversion center (Fig. 1). It consists of eight edge-sharing $MoO_6$ octahedra and displays the characteristic β-octamolybdate arrangement. Through N—H···O hydrogen bonds each protonated $[H_2L]^{2+}$ cation is linked two $[Mo_8O_{26}]^{4-}$ anions, and each $[Mo_8O_{26}]^{4-}$ anion joins four protonated $[H_2L]^{2+}$ cations (see the hydrogen bonding table for numerical values). The hydrogen bonds in the title compound thus create a two-dimensional supramolecular layerlike structure (Fig. 2).

## Experimental

A mixture of $Na_2MoO_4{\cdot}2H_2O$ (0.242 g, 1.0 mmol) and *L* (0.316 g, 1.0 mmol) in water (10 ml) was adjusted with HCl (6*M*) to pH = 2. Then the mixture was placed in a 23 ml Teflon-lined autoclave and kept under autogenous pressure at 150 °C for 3 days. After the mixture was cooled to room temperature at 10°C $h^{-1}$, colorless crystals of the title compound were obtained.

## Refinement

All H atoms on C atoms were poisitioned geometrically and refined as riding atoms, with C—H = 0.93 − 0.97 Å, and $U_{iso}$=1.2$U_{eq}$ (C). The H atoms of N5 and N6 were located in a difference Fourier map and then refined isotropically.

## Figures

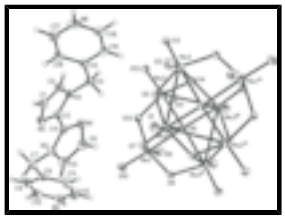

Fig. 1. A view of the molecule of the title compound. Displacement ellipsoids are drawn at the 30% probability level. Symmetry code: (iii) 1 − *x*, −*y*, −*z*. Oxygen atom created by the inversion center are unlabled for clarity.

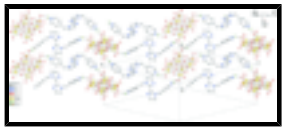

Fig. 2. Ball and stick representation of the two-dimensional supramolecular structure of the title compound.

**bis{4,4'-[(2,2'-bi-1*H*-imidazole-1,1'-diyl)dimethylene]dipyridinium} β-octamolybdate**

*Crystal data*

| | |
|---|---|
| $(C_{18}H_{18}N_6)_2[Mo_8O_{26}]$ | $Z = 4$ |
| $M_r = 1820.28$ | $F_{000} = 3520$ |
| Monoclinic, $C2/c$ | $D_x = 2.368$ Mg m$^{-3}$ |
| Hall symbol: -C2yc | Mo $K\alpha$ radiation<br>$\lambda = 0.71069$ Å |
| $a = 23.1640$ (4) Å | $\theta = 1.9$–$28.3$º |
| $b = 10.4740$ (5) Å | $\mu = 2.00$ mm$^{-1}$ |
| $c = 22.7770$ (8) Å | $T = 293$ (2) K |
| $\beta = 112.4940$ (10)º | Block, colorless |
| $V = 5105.7$ (3) Å$^3$ | 0.28 × 0.26 × 0.19 mm |

*Data collection*

| | |
|---|---|
| Bruker APEX CCD area-detector diffractometer | 6141 independent reflections |
| Radiation source: fine-focus sealed tube | 5242 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.020$ |
| $T = 293$(2) K | $\theta_{max} = 28.3$º |
| ω scans | $\theta_{min} = 1.9$º |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h = -29\rightarrow30$ |
| $T_{min} = 0.481$, $T_{max} = 0.684$ | $k = -13\rightarrow8$ |
| 15475 measured reflections | $l = -29\rightarrow28$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.023$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.054$ | $w = 1/[\sigma^2(F_o^2) + (0.0237P)^2 + 2.9429P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.02$ | $(\Delta/\sigma)_{max} = 0.003$ |
| 6141 reflections | $\Delta\rho_{max} = 0.32$ e Å$^{-3}$ |
| 378 parameters | $\Delta\rho_{min} = -0.48$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.89870 (14) | −0.0869 (3) | 0.27475 (14) | 0.0441 (7) |
| H1 | 0.9358 | −0.1323 | 0.2928 | 0.053* |
| C2 | 0.84466 (13) | −0.1193 (3) | 0.28019 (13) | 0.0405 (7) |
| H2 | 0.8379 | −0.1887 | 0.3022 | 0.049* |
| C12 | 0.87836 (16) | 0.0072 (3) | 0.03172 (16) | 0.0545 (8) |
| H12 | 0.8468 | −0.0268 | −0.0039 | 0.065* |
| C3 | 0.83246 (12) | 0.0547 (2) | 0.22249 (12) | 0.0315 (6) |
| C4 | 0.80217 (12) | 0.1615 (2) | 0.18149 (12) | 0.0322 (6) |
| C5 | 0.78785 (14) | 0.3224 (3) | 0.11565 (13) | 0.0402 (7) |
| H5 | 0.7941 | 0.3871 | 0.0907 | 0.048* |
| C6 | 0.73332 (14) | 0.2882 (3) | 0.11943 (13) | 0.0411 (7) |
| H6 | 0.6950 | 0.3267 | 0.0968 | 0.049* |
| C7 | 0.89781 (12) | 0.2422 (3) | 0.16363 (14) | 0.0378 (6) |
| H7A | 0.9237 | 0.2246 | 0.2077 | 0.045* |
| H7B | 0.9089 | 0.3262 | 0.1533 | 0.045* |
| C8 | 0.91118 (12) | 0.1443 (2) | 0.12192 (12) | 0.0325 (6) |
| C9 | 0.97181 (14) | 0.1054 (3) | 0.13511 (14) | 0.0427 (7) |
| H9 | 1.0045 | 0.1378 | 0.1702 | 0.051* |
| C10 | 0.98359 (15) | 0.0179 (3) | 0.09575 (16) | 0.0483 (8) |
| H10 | 1.0243 | −0.0082 | 0.1041 | 0.058* |
| C11 | 0.86399 (14) | 0.0944 (3) | 0.06898 (15) | 0.0466 (7) |
| H11 | 0.8228 | 0.1197 | 0.0587 | 0.056* |
| C13 | 0.73548 (12) | −0.0334 (3) | 0.23536 (12) | 0.0336 (6) |
| H13A | 0.7248 | −0.1209 | 0.2410 | 0.040* |
| H13B | 0.7117 | −0.0102 | 0.1915 | 0.040* |
| C14 | 0.71528 (12) | 0.0512 (2) | 0.27743 (12) | 0.0316 (6) |
| C15 | 0.65174 (13) | 0.0563 (3) | 0.26529 (13) | 0.0385 (6) |
| H15 | 0.6234 | 0.0126 | 0.2307 | 0.046* |
| C16 | 0.63082 (16) | 0.1256 (3) | 0.30408 (15) | 0.0503 (8) |
| H16 | 0.5883 | 0.1298 | 0.2959 | 0.060* |
| C17 | 0.7328 (2) | 0.1859 (3) | 0.36671 (16) | 0.0633 (10) |
| H17 | 0.7600 | 0.2301 | 0.4018 | 0.076* |
| C18 | 0.75615 (15) | 0.1192 (3) | 0.32810 (14) | 0.0486 (8) |

| | | | | |
|---|---|---|---|---|
| H18 | 0.7987 | 0.1203 | 0.3362 | 0.058* |
| N1 | 0.74194 (10) | 0.1887 (2) | 0.16133 (11) | 0.0384 (5) |
| N2 | 0.83244 (10) | 0.2425 (2) | 0.15601 (11) | 0.0345 (5) |
| N3 | 0.80131 (10) | −0.0286 (2) | 0.24644 (10) | 0.0329 (5) |
| N4 | 0.89177 (11) | 0.0223 (2) | 0.23895 (11) | 0.0409 (6) |
| N5 | 0.93715 (14) | −0.0286 (3) | 0.04640 (14) | 0.0485 (7) |
| N6 | 0.67189 (17) | 0.1870 (3) | 0.35373 (15) | 0.0588 (8) |
| O1 | 0.54584 (8) | 0.29320 (16) | 0.04539 (8) | 0.0358 (4) |
| O2 | 0.48100 (9) | 0.19921 (19) | 0.13672 (10) | 0.0456 (5) |
| O3 | 0.50867 (8) | −0.0374 (2) | 0.18620 (8) | 0.0414 (5) |
| O4 | 0.49368 (7) | −0.15179 (15) | 0.06816 (7) | 0.0262 (4) |
| O5 | 0.56402 (7) | 0.04669 (16) | 0.10224 (7) | 0.0265 (4) |
| O6 | 0.54342 (7) | −0.07885 (15) | −0.01015 (7) | 0.0253 (4) |
| O7 | 0.62419 (7) | 0.12170 (16) | 0.02375 (8) | 0.0296 (4) |
| O8 | 0.60282 (8) | −0.00043 (17) | −0.08372 (8) | 0.0297 (4) |
| O9 | 0.65482 (9) | −0.22313 (19) | −0.02666 (9) | 0.0443 (5) |
| O10 | 0.72562 (8) | −0.0123 (2) | 0.00907 (9) | 0.0466 (5) |
| O11 | 0.58417 (9) | −0.32189 (17) | 0.06189 (9) | 0.0377 (4) |
| O12 | 0.61036 (8) | −0.18874 (17) | 0.17013 (8) | 0.0359 (4) |
| O13 | 0.65713 (8) | −0.10327 (17) | 0.08166 (8) | 0.0313 (4) |
| Mo1 | 0.653779 (10) | −0.06854 (2) | −0.002152 (10) | 0.03034 (6) |
| Mo2 | 0.584432 (10) | −0.17049 (2) | 0.090220 (10) | 0.02619 (6) |
| Mo3 | 0.549524 (9) | 0.139409 (19) | 0.023708 (9) | 0.02377 (6) |
| Mo4 | 0.484198 (10) | 0.04345 (2) | 0.116550 (10) | 0.02825 (6) |
| H5N | 0.9441 (15) | −0.079 (3) | 0.0245 (15) | 0.052 (10)* |
| H6N | 0.6554 (17) | 0.225 (4) | 0.3730 (17) | 0.070 (12)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0370 (16) | 0.0398 (16) | 0.0520 (18) | 0.0077 (13) | 0.0130 (14) | 0.0042 (14) |
| C2 | 0.0447 (17) | 0.0339 (14) | 0.0431 (16) | 0.0005 (13) | 0.0172 (14) | 0.0047 (12) |
| C12 | 0.052 (2) | 0.0518 (19) | 0.054 (2) | −0.0037 (16) | 0.0147 (16) | −0.0143 (16) |
| C3 | 0.0297 (13) | 0.0293 (13) | 0.0369 (14) | −0.0029 (11) | 0.0144 (11) | −0.0021 (11) |
| C4 | 0.0350 (14) | 0.0302 (13) | 0.0347 (14) | −0.0015 (11) | 0.0170 (12) | −0.0036 (11) |
| C5 | 0.0508 (18) | 0.0310 (14) | 0.0418 (16) | 0.0035 (13) | 0.0209 (14) | 0.0030 (12) |
| C6 | 0.0415 (16) | 0.0368 (15) | 0.0417 (16) | 0.0049 (13) | 0.0124 (13) | 0.0026 (12) |
| C7 | 0.0340 (15) | 0.0334 (14) | 0.0504 (17) | −0.0053 (12) | 0.0210 (13) | −0.0030 (12) |
| C8 | 0.0348 (14) | 0.0276 (13) | 0.0395 (15) | −0.0044 (11) | 0.0193 (12) | 0.0027 (11) |
| C9 | 0.0388 (16) | 0.0433 (17) | 0.0463 (17) | 0.0006 (13) | 0.0167 (14) | 0.0015 (14) |
| C10 | 0.0465 (18) | 0.0465 (18) | 0.060 (2) | 0.0088 (15) | 0.0302 (17) | 0.0102 (16) |
| C11 | 0.0364 (16) | 0.0445 (17) | 0.0553 (19) | −0.0026 (13) | 0.0135 (14) | −0.0104 (15) |
| C13 | 0.0322 (14) | 0.0353 (14) | 0.0350 (14) | −0.0065 (11) | 0.0148 (12) | −0.0032 (11) |
| C14 | 0.0351 (14) | 0.0337 (13) | 0.0269 (13) | −0.0065 (11) | 0.0129 (11) | 0.0015 (10) |
| C15 | 0.0368 (15) | 0.0476 (17) | 0.0326 (15) | −0.0007 (13) | 0.0151 (12) | 0.0020 (12) |
| C16 | 0.057 (2) | 0.0530 (19) | 0.0518 (19) | 0.0047 (16) | 0.0328 (17) | 0.0121 (16) |
| C17 | 0.090 (3) | 0.054 (2) | 0.050 (2) | −0.029 (2) | 0.032 (2) | −0.0212 (16) |
| C18 | 0.0483 (18) | 0.0533 (19) | 0.0460 (18) | −0.0195 (15) | 0.0201 (15) | −0.0128 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N1 | 0.0347 (13) | 0.0393 (13) | 0.0417 (13) | 0.0039 (10) | 0.0152 (11) | 0.0017 (10) |
| N2 | 0.0354 (12) | 0.0281 (11) | 0.0466 (13) | −0.0002 (10) | 0.0228 (11) | 0.0003 (10) |
| N3 | 0.0330 (12) | 0.0308 (11) | 0.0361 (12) | −0.0041 (9) | 0.0146 (10) | −0.0018 (9) |
| N4 | 0.0344 (13) | 0.0374 (13) | 0.0524 (15) | 0.0018 (10) | 0.0184 (11) | 0.0038 (11) |
| N5 | 0.0660 (19) | 0.0373 (14) | 0.0538 (17) | 0.0026 (13) | 0.0357 (16) | −0.0050 (13) |
| N6 | 0.093 (3) | 0.0454 (16) | 0.063 (2) | −0.0071 (16) | 0.058 (2) | −0.0098 (14) |
| O1 | 0.0408 (11) | 0.0279 (9) | 0.0389 (10) | −0.0042 (8) | 0.0155 (9) | −0.0040 (8) |
| O2 | 0.0472 (12) | 0.0439 (12) | 0.0516 (12) | −0.0061 (9) | 0.0253 (10) | −0.0137 (10) |
| O3 | 0.0334 (10) | 0.0642 (13) | 0.0275 (10) | −0.0030 (9) | 0.0127 (8) | 0.0045 (9) |
| O4 | 0.0249 (9) | 0.0288 (9) | 0.0237 (8) | −0.0023 (7) | 0.0080 (7) | 0.0039 (7) |
| O5 | 0.0238 (8) | 0.0334 (9) | 0.0209 (8) | −0.0026 (7) | 0.0069 (7) | 0.0006 (7) |
| O6 | 0.0222 (8) | 0.0283 (8) | 0.0248 (9) | −0.0011 (7) | 0.0082 (7) | 0.0016 (7) |
| O7 | 0.0231 (9) | 0.0346 (9) | 0.0295 (9) | −0.0044 (7) | 0.0082 (7) | 0.0002 (7) |
| O8 | 0.0257 (9) | 0.0386 (10) | 0.0266 (9) | −0.0013 (8) | 0.0120 (7) | 0.0029 (8) |
| O9 | 0.0540 (13) | 0.0415 (11) | 0.0438 (11) | 0.0116 (10) | 0.0259 (10) | 0.0066 (9) |
| O10 | 0.0281 (10) | 0.0668 (14) | 0.0460 (12) | 0.0000 (10) | 0.0153 (9) | 0.0103 (11) |
| O11 | 0.0397 (11) | 0.0322 (10) | 0.0408 (11) | 0.0028 (8) | 0.0149 (9) | −0.0013 (8) |
| O12 | 0.0336 (10) | 0.0447 (11) | 0.0261 (9) | −0.0011 (8) | 0.0079 (8) | 0.0070 (8) |
| O13 | 0.0242 (9) | 0.0398 (10) | 0.0277 (9) | 0.0014 (8) | 0.0074 (7) | 0.0063 (8) |
| Mo1 | 0.02537 (12) | 0.03820 (13) | 0.02936 (12) | 0.00348 (9) | 0.01259 (9) | 0.00555 (9) |
| Mo2 | 0.02420 (11) | 0.02897 (11) | 0.02414 (11) | 0.00120 (9) | 0.00783 (9) | 0.00379 (8) |
| Mo3 | 0.02227 (11) | 0.02433 (10) | 0.02358 (11) | −0.00386 (8) | 0.00752 (8) | −0.00023 (8) |
| Mo4 | 0.02511 (11) | 0.03664 (12) | 0.02427 (11) | −0.00324 (9) | 0.01086 (9) | −0.00291 (9) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.348 (4) | C16—H16 | 0.9300 |
| C1—N4 | 1.378 (4) | C17—N6 | 1.327 (5) |
| C1—H1 | 0.9300 | C17—C18 | 1.384 (4) |
| C2—N3 | 1.382 (3) | C17—H17 | 0.9300 |
| C2—H2 | 0.9300 | C18—H18 | 0.9300 |
| C12—N5 | 1.326 (4) | N5—H5N | 0.79 (3) |
| C12—C11 | 1.371 (4) | N6—H6N | 0.79 (3) |
| C12—H12 | 0.9300 | O1—Mo3 | 1.6964 (17) |
| C3—N4 | 1.323 (3) | O2—Mo4 | 1.7042 (19) |
| C3—N3 | 1.372 (3) | O3—Mo4 | 1.6934 (18) |
| C3—C4 | 1.454 (4) | O4—Mo3$^{i}$ | 1.9479 (16) |
| C4—N1 | 1.322 (3) | O4—Mo2 | 1.9753 (16) |
| C4—N2 | 1.364 (3) | O4—Mo4 | 2.3728 (16) |
| C5—C6 | 1.347 (4) | O5—Mo3 | 1.9483 (16) |
| C5—N2 | 1.373 (3) | O5—Mo4 | 1.9967 (16) |
| C5—H5 | 0.9300 | O5—Mo2 | 2.3605 (17) |
| C6—N1 | 1.376 (3) | O6—Mo3$^{i}$ | 2.1503 (15) |
| C6—H6 | 0.9300 | O6—Mo4$^{i}$ | 2.2878 (15) |
| C7—N2 | 1.457 (3) | O6—Mo2 | 2.3212 (15) |
| C7—C8 | 1.508 (4) | O6—Mo3 | 2.3995 (16) |
| C7—H7A | 0.9700 | O6—Mo1 | 2.4948 (16) |
| C7—H7B | 0.9700 | O7—Mo3 | 1.7390 (16) |

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|---|---|---|---|
| C8—C9 | 1.381 (4) | O7—Mo1 | 2.2578 (17) |
| C8—C11 | 1.383 (4) | O8—Mo4$^{i}$ | 1.9163 (16) |
| C9—C10 | 1.380 (4) | O8—Mo1 | 1.9172 (16) |
| C9—H9 | 0.9300 | O9—Mo1 | 1.716 (2) |
| C10—N5 | 1.316 (4) | O10—Mo1 | 1.6902 (19) |
| C10—H10 | 0.9300 | O11—Mo2 | 1.7111 (18) |
| C11—H11 | 0.9300 | O12—Mo2 | 1.6952 (17) |
| C13—N3 | 1.448 (3) | O13—Mo2 | 1.9028 (17) |
| C13—C14 | 1.506 (4) | O13—Mo1 | 1.9155 (17) |
| C13—H13A | 0.9700 | Mo2—Mo3$^{i}$ | 3.2104 (3) |
| C13—H13B | 0.9700 | Mo3—O4$^{i}$ | 1.9479 (16) |
| C14—C18 | 1.378 (4) | Mo3—O6$^{i}$ | 2.1503 (15) |
| C14—C15 | 1.391 (4) | Mo3—Mo4 | 3.1969 (3) |
| C15—C16 | 1.367 (4) | Mo3—Mo2$^{i}$ | 3.2104 (3) |
| C15—H15 | 0.9300 | Mo4—O8$^{i}$ | 1.9163 (16) |
| C16—N6 | 1.332 (4) | Mo4—O6$^{i}$ | 2.2878 (15) |
| C2—C1—N4 | 111.2 (3) | Mo3—O6—Mo1 | 90.14 (5) |
| C2—C1—H1 | 124.4 | Mo3—O7—Mo1 | 119.69 (8) |
| N4—C1—H1 | 124.4 | Mo4$^{i}$—O8—Mo1 | 117.16 (8) |
| C1—C2—N3 | 106.2 (2) | Mo2—O13—Mo1 | 118.19 (8) |
| C1—C2—H2 | 126.9 | O10—Mo1—O9 | 104.05 (10) |
| N3—C2—H2 | 126.9 | O10—Mo1—O13 | 104.68 (8) |
| N5—C12—C11 | 120.1 (3) | O9—Mo1—O13 | 98.32 (8) |
| N5—C12—H12 | 120.0 | O10—Mo1—O8 | 102.85 (8) |
| C11—C12—H12 | 120.0 | O9—Mo1—O8 | 96.66 (8) |
| N4—C3—N3 | 111.8 (2) | O13—Mo1—O8 | 144.25 (7) |
| N4—C3—C4 | 125.0 (2) | O10—Mo1—O7 | 91.86 (8) |
| N3—C3—C4 | 123.2 (2) | O9—Mo1—O7 | 164.00 (8) |
| N1—C4—N2 | 111.4 (2) | O13—Mo1—O7 | 78.92 (7) |
| N1—C4—C3 | 125.0 (2) | O8—Mo1—O7 | 77.81 (7) |
| N2—C4—C3 | 123.5 (2) | O10—Mo1—O6 | 161.50 (8) |
| C6—C5—N2 | 106.2 (2) | O9—Mo1—O6 | 94.41 (8) |
| C6—C5—H5 | 126.9 | O13—Mo1—O6 | 73.39 (6) |
| N2—C5—H5 | 126.9 | O8—Mo1—O6 | 73.24 (6) |
| C5—C6—N1 | 110.8 (3) | O7—Mo1—O6 | 69.65 (5) |
| C5—C6—H6 | 124.6 | O12—Mo2—O11 | 104.42 (9) |
| N1—C6—H6 | 124.6 | O12—Mo2—O13 | 100.83 (8) |
| N2—C7—C8 | 112.4 (2) | O11—Mo2—O13 | 100.36 (8) |
| N2—C7—H7A | 109.1 | O12—Mo2—O4 | 100.93 (8) |
| C8—C7—H7A | 109.1 | O11—Mo2—O4 | 98.40 (8) |
| N2—C7—H7B | 109.1 | O13—Mo2—O4 | 146.58 (7) |
| C8—C7—H7B | 109.1 | O12—Mo2—O6 | 161.34 (8) |
| H7A—C7—H7B | 107.9 | O11—Mo2—O6 | 94.06 (7) |
| C9—C8—C11 | 118.5 (3) | O13—Mo2—O6 | 77.93 (6) |
| C9—C8—C7 | 120.0 (2) | O4—Mo2—O6 | 73.36 (6) |
| C11—C8—C7 | 121.5 (2) | O12—Mo2—O5 | 89.34 (7) |
| C10—C9—C8 | 119.5 (3) | O11—Mo2—O5 | 164.76 (7) |

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| C10—C9—H9 | 120.3 | O13—Mo2—O5 | 83.09 (7) |
| C8—C9—H9 | 120.3 | O4—Mo2—O5 | 72.12 (6) |
| N5—C10—C9 | 120.0 (3) | O6—Mo2—O5 | 72.01 (5) |
| N5—C10—H10 | 120.0 | O12—Mo2—Mo3$^{i}$ | 135.65 (6) |
| C9—C10—H10 | 120.0 | O11—Mo2—Mo3$^{i}$ | 85.77 (6) |
| C12—C11—C8 | 119.6 (3) | O13—Mo2—Mo3$^{i}$ | 119.95 (5) |
| C12—C11—H11 | 120.2 | O4—Mo2—Mo3$^{i}$ | 34.80 (5) |
| C8—C11—H11 | 120.2 | O6—Mo2—Mo3$^{i}$ | 42.03 (4) |
| N3—C13—C14 | 115.6 (2) | O5—Mo2—Mo3$^{i}$ | 79.71 (4) |
| N3—C13—H13A | 108.4 | O1—Mo3—O7 | 105.18 (8) |
| C14—C13—H13A | 108.4 | O1—Mo3—O4$^{i}$ | 100.78 (8) |
| N3—C13—H13B | 108.4 | O7—Mo3—O4$^{i}$ | 96.30 (7) |
| C14—C13—H13B | 108.4 | O1—Mo3—O5 | 102.49 (8) |
| H13A—C13—H13B | 107.5 | O7—Mo3—O5 | 97.14 (7) |
| C18—C14—C15 | 118.8 (3) | O4$^{i}$—Mo3—O5 | 148.94 (7) |
| C18—C14—C13 | 123.8 (3) | O1—Mo3—O6$^{i}$ | 99.37 (8) |
| C15—C14—C13 | 117.3 (2) | O7—Mo3—O6$^{i}$ | 155.43 (7) |
| C16—C15—C14 | 120.1 (3) | O4$^{i}$—Mo3—O6$^{i}$ | 77.92 (6) |
| C16—C15—H15 | 119.9 | O5—Mo3—O6$^{i}$ | 78.24 (6) |
| C14—C15—H15 | 119.9 | O1—Mo3—O6 | 174.18 (7) |
| N6—C16—C15 | 119.4 (3) | O7—Mo3—O6 | 80.50 (7) |
| N6—C16—H16 | 120.3 | O4$^{i}$—Mo3—O6 | 77.02 (6) |
| C15—C16—H16 | 120.3 | O5—Mo3—O6 | 77.78 (6) |
| N6—C17—C18 | 120.2 (3) | O6$^{i}$—Mo3—O6 | 74.94 (6) |
| N6—C17—H17 | 119.9 | O1—Mo3—Mo4 | 90.96 (6) |
| C18—C17—H17 | 119.9 | O7—Mo3—Mo4 | 133.50 (6) |
| C14—C18—C17 | 118.9 (3) | O4$^{i}$—Mo3—Mo4 | 123.56 (5) |
| C14—C18—H18 | 120.6 | O5—Mo3—Mo4 | 36.38 (5) |
| C17—C18—H18 | 120.6 | O6$^{i}$—Mo3—Mo4 | 45.65 (4) |
| C4—N1—C6 | 104.9 (2) | O6—Mo3—Mo4 | 85.89 (4) |
| C4—N2—C5 | 106.7 (2) | O1—Mo3—Mo2$^{i}$ | 89.91 (6) |
| C4—N2—C7 | 128.9 (2) | O7—Mo3—Mo2$^{i}$ | 131.66 (5) |
| C5—N2—C7 | 124.2 (2) | O4$^{i}$—Mo3—Mo2$^{i}$ | 35.37 (5) |
| C3—N3—C2 | 106.1 (2) | O5—Mo3—Mo2$^{i}$ | 124.50 (5) |
| C3—N3—C13 | 129.2 (2) | O6$^{i}$—Mo3—Mo2$^{i}$ | 46.28 (4) |
| C2—N3—C13 | 124.4 (2) | O6—Mo3—Mo2$^{i}$ | 85.24 (4) |
| C3—N4—C1 | 104.7 (2) | Mo4—Mo3—Mo2$^{i}$ | 90.620 (8) |
| C10—N5—C12 | 122.4 (3) | O3—Mo4—O2 | 105.07 (10) |
| C10—N5—H5N | 120 (2) | O3—Mo4—O8$^{i}$ | 99.97 (8) |
| C12—N5—H5N | 118 (2) | O2—Mo4—O8$^{i}$ | 100.52 (9) |
| C17—N6—C16 | 122.5 (3) | O3—Mo4—O5 | 99.35 (8) |
| C17—N6—H6N | 125 (3) | O2—Mo4—O5 | 99.57 (8) |
| C16—N6—H6N | 112 (3) | O8$^{i}$—Mo4—O5 | 147.33 (7) |

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| Mo3$^{i}$—O4—Mo2 | 109.83 (8) | O3—Mo4—O6$^{i}$ | 158.62 (8) |
| Mo3$^{i}$—O4—Mo4 | 109.92 (7) | O2—Mo4—O6$^{i}$ | 96.14 (8) |
| Mo2—O4—Mo4 | 104.24 (7) | O8$^{i}$—Mo4—O6$^{i}$ | 78.38 (6) |
| Mo3—O5—Mo4 | 108.26 (7) | O5—Mo4—O6$^{i}$ | 74.06 (6) |
| Mo3—O5—Mo2 | 110.22 (7) | O3—Mo4—O4 | 86.94 (8) |
| Mo4—O5—Mo2 | 103.99 (7) | O2—Mo4—O4 | 166.31 (8) |
| Mo3$^{i}$—O6—Mo4$^{i}$ | 92.11 (6) | O8$^{i}$—Mo4—O4 | 83.49 (7) |
| Mo3$^{i}$—O6—Mo2 | 91.69 (6) | O5—Mo4—O4 | 71.51 (6) |
| Mo4$^{i}$—O6—Mo2 | 162.46 (8) | O6$^{i}$—Mo4—O4 | 71.68 (6) |
| Mo3$^{i}$—O6—Mo3 | 105.06 (6) | O3—Mo4—Mo3 | 134.70 (6) |
| Mo4$^{i}$—O6—Mo3 | 98.29 (6) | O2—Mo4—Mo3 | 87.58 (7) |
| Mo2—O6—Mo3 | 97.23 (6) | O8$^{i}$—Mo4—Mo3 | 120.61 (5) |
| Mo3$^{i}$—O6—Mo1 | 164.78 (8) | O5—Mo4—Mo3 | 35.36 (5) |
| Mo4$^{i}$—O6—Mo1 | 86.20 (5) | O6$^{i}$—Mo4—Mo3 | 42.23 (4) |
| Mo2—O6—Mo1 | 85.65 (5) | O4—Mo4—Mo3 | 79.18 (4) |
| N4—C1—C2—N3 | 0.4 (3) | Mo3—O6—Mo2—Mo3$^{i}$ | 105.42 (7) |
| N4—C3—C4—N1 | 174.9 (3) | Mo1—O6—Mo2—Mo3$^{i}$ | −164.99 (8) |
| N3—C3—C4—N1 | −1.9 (4) | Mo3—O5—Mo2—O12 | 166.34 (9) |
| N4—C3—C4—N2 | −1.2 (4) | Mo4—O5—Mo2—O12 | −77.83 (8) |
| N3—C3—C4—N2 | −178.0 (2) | Mo3—O5—Mo2—O11 | −38.8 (3) |
| N2—C5—C6—N1 | 0.2 (3) | Mo4—O5—Mo2—O11 | 77.0 (3) |
| N2—C7—C8—C9 | −161.8 (2) | Mo3—O5—Mo2—O13 | 65.35 (8) |
| N2—C7—C8—C11 | 20.1 (4) | Mo4—O5—Mo2—O13 | −178.82 (8) |
| C11—C8—C9—C10 | −0.4 (4) | Mo3—O5—Mo2—O4 | −91.95 (8) |
| C7—C8—C9—C10 | −178.5 (3) | Mo4—O5—Mo2—O4 | 23.89 (6) |
| C8—C9—C10—N5 | −0.6 (4) | Mo3—O5—Mo2—O6 | −14.16 (7) |
| N5—C12—C11—C8 | −0.1 (5) | Mo4—O5—Mo2—O6 | 101.68 (7) |
| C9—C8—C11—C12 | 0.7 (4) | Mo3—O5—Mo2—Mo3$^{i}$ | −56.87 (6) |
| C7—C8—C11—C12 | 178.8 (3) | Mo4—O5—Mo2—Mo3$^{i}$ | 58.97 (5) |
| N3—C13—C14—C18 | −7.0 (4) | Mo1—O7—Mo3—O1 | 179.96 (9) |
| N3—C13—C14—C15 | 175.5 (2) | Mo1—O7—Mo3—O4$^{i}$ | −77.03 (10) |
| C18—C14—C15—C16 | −1.4 (4) | Mo1—O7—Mo3—O5 | 74.91 (9) |
| C13—C14—C15—C16 | 176.2 (2) | Mo1—O7—Mo3—O6$^{i}$ | −2.4 (2) |
| C14—C15—C16—N6 | −0.5 (4) | Mo1—O7—Mo3—O6 | −1.37 (8) |
| C15—C14—C18—C17 | 2.7 (4) | Mo1—O7—Mo3—Mo4 | 73.62 (11) |
| C13—C14—C18—C17 | −174.8 (3) | Mo1—O7—Mo3—Mo2$^{i}$ | −76.20 (10) |
| N6—C17—C18—C14 | −2.0 (5) | Mo4—O5—Mo3—O1 | 74.24 (9) |
| N2—C4—N1—C6 | 2.3 (3) | Mo2—O5—Mo3—O1 | −172.64 (8) |
| C3—C4—N1—C6 | −174.3 (3) | Mo4—O5—Mo3—O7 | −178.43 (8) |
| C5—C6—N1—C4 | −1.5 (3) | Mo2—O5—Mo3—O7 | −65.30 (8) |
| N1—C4—N2—C5 | −2.2 (3) | Mo4—O5—Mo3—O4$^{i}$ | −63.43 (16) |
| C3—C4—N2—C5 | 174.4 (2) | Mo2—O5—Mo3—O4$^{i}$ | 49.69 (16) |
| N1—C4—N2—C7 | −177.1 (2) | Mo4—O5—Mo3—O6$^{i}$ | −22.90 (7) |
| C3—C4—N2—C7 | −0.5 (4) | Mo2—O5—Mo3—O6$^{i}$ | 90.22 (7) |

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| C6—C5—N2—C4 | 1.2 (3) | Mo4—O5—Mo3—O6 | −99.81 (8) |
| C6—C5—N2—C7 | 176.4 (2) | Mo2—O5—Mo3—O6 | 13.31 (6) |
| C8—C7—N2—C4 | 79.5 (3) | Mo2—O5—Mo3—Mo4 | 113.12 (10) |
| C8—C7—N2—C5 | −94.6 (3) | Mo4—O5—Mo3—Mo2$^{i}$ | −24.40 (10) |
| N4—C3—N3—C2 | 0.0 (3) | Mo2—O5—Mo3—Mo2$^{i}$ | 88.72 (7) |
| C4—C3—N3—C2 | 177.2 (2) | Mo3$^{i}$—O6—Mo3—O7 | −179.56 (8) |
| N4—C3—N3—C13 | −174.4 (2) | Mo4$^{i}$—O6—Mo3—O7 | −85.10 (7) |
| C4—C3—N3—C13 | 2.8 (4) | Mo2—O6—Mo3—O7 | 86.71 (7) |
| C1—C2—N3—C3 | −0.2 (3) | Mo1—O6—Mo3—O7 | 1.08 (6) |
| C1—C2—N3—C13 | 174.5 (2) | Mo3$^{i}$—O6—Mo3—O4$^{i}$ | −80.77 (7) |
| C14—C13—N3—C3 | −85.4 (3) | Mo4$^{i}$—O6—Mo3—O4$^{i}$ | 13.69 (6) |
| C14—C13—N3—C2 | 101.1 (3) | Mo2—O6—Mo3—O4$^{i}$ | −174.50 (7) |
| N3—C3—N4—C1 | 0.3 (3) | Mo1—O6—Mo3—O4$^{i}$ | 99.87 (6) |
| C4—C3—N4—C1 | −176.9 (3) | Mo3$^{i}$—O6—Mo3—O5 | 80.93 (7) |
| C2—C1—N4—C3 | −0.4 (3) | Mo4$^{i}$—O6—Mo3—O5 | 175.39 (7) |
| C9—C10—N5—C12 | 1.3 (5) | Mo2—O6—Mo3—O5 | −12.80 (6) |
| C11—C12—N5—C10 | −1.0 (5) | Mo1—O6—Mo3—O5 | −98.43 (6) |
| C18—C17—N6—C16 | 0.0 (5) | Mo3$^{i}$—O6—Mo3—O6$^{i}$ | 0.0 |
| C15—C16—N6—C17 | 1.3 (5) | Mo4$^{i}$—O6—Mo3—O6$^{i}$ | 94.46 (7) |
| Mo2—O13—Mo1—O10 | −179.55 (10) | Mo2—O6—Mo3—O6$^{i}$ | −93.73 (7) |
| Mo2—O13—Mo1—O9 | −72.58 (11) | Mo1—O6—Mo3—O6$^{i}$ | −179.36 (9) |
| Mo2—O13—Mo1—O8 | 41.23 (18) | Mo3$^{i}$—O6—Mo3—Mo4 | 45.06 (5) |
| Mo2—O13—Mo1—O7 | 91.42 (10) | Mo4$^{i}$—O6—Mo3—Mo4 | 139.52 (5) |
| Mo2—O13—Mo1—O6 | 19.57 (8) | Mo2—O6—Mo3—Mo4 | −48.67 (4) |
| Mo4$^{i}$—O8—Mo1—O10 | 179.11 (10) | Mo1—O6—Mo3—Mo4 | −134.30 (4) |
| Mo4$^{i}$—O8—Mo1—O9 | 73.01 (11) | Mo3$^{i}$—O6—Mo3—Mo2$^{i}$ | −45.91 (5) |
| Mo4$^{i}$—O8—Mo1—O13 | −41.29 (18) | Mo4$^{i}$—O6—Mo3—Mo2$^{i}$ | 48.55 (4) |
| Mo4$^{i}$—O8—Mo1—O7 | −91.75 (10) | Mo2—O6—Mo3—Mo2$^{i}$ | −139.64 (5) |
| Mo4$^{i}$—O8—Mo1—O6 | −19.61 (8) | Mo1—O6—Mo3—Mo2$^{i}$ | 134.73 (4) |
| Mo3—O7—Mo1—O10 | −179.44 (10) | Mo3—O5—Mo4—O3 | −179.00 (9) |
| Mo3—O7—Mo1—O9 | 6.6 (3) | Mo2—O5—Mo4—O3 | 63.79 (9) |
| Mo3—O7—Mo1—O13 | −74.85 (10) | Mo3—O5—Mo4—O2 | −71.85 (10) |
| Mo3—O7—Mo1—O8 | 77.82 (10) | Mo2—O5—Mo4—O2 | 170.94 (8) |
| Mo3—O7—Mo1—O6 | 1.39 (8) | Mo3—O5—Mo4—O8$^{i}$ | 55.44 (16) |
| Mo3$^{i}$—O6—Mo1—O10 | 178.9 (3) | Mo2—O5—Mo4—O8$^{i}$ | −61.77 (14) |
| Mo4$^{i}$—O6—Mo1—O10 | 94.8 (2) | Mo3—O5—Mo4—O6$^{i}$ | 21.86 (7) |
| Mo2—O6—Mo1—O10 | −100.7 (2) | Mo2—O5—Mo4—O6$^{i}$ | −95.35 (7) |
| Mo3—O6—Mo1—O10 | −3.5 (3) | Mo3—O5—Mo4—O4 | 97.44 (8) |
| Mo3$^{i}$—O6—Mo1—O9 | 2.9 (3) | Mo2—O5—Mo4—O4 | −19.77 (5) |
| Mo4$^{i}$—O6—Mo1—O9 | −81.12 (8) | Mo2—O5—Mo4—Mo3 | −117.21 (10) |
| Mo2—O6—Mo1—O9 | 83.34 (7) | Mo3$^{i}$—O4—Mo4—O3 | 165.30 (9) |
| Mo3—O6—Mo1—O9 | −179.42 (7) | Mo2—O4—Mo4—O3 | −77.04 (8) |
| Mo3$^{i}$—O6—Mo1—O13 | −94.4 (3) | Mo3$^{i}$—O4—Mo4—O2 | −43.0 (4) |

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| Mo4$^{i}$—O6—Mo1—O13 | −178.50 (7) | Mo2—O4—Mo4—O2 | 74.6 (3) |
| Mo2—O6—Mo1—O13 | −14.04 (6) | Mo3$^{i}$—O4—Mo4—O8$^{i}$ | 64.90 (8) |
| Mo3—O6—Mo1—O13 | 83.20 (7) | Mo2—O4—Mo4—O8$^{i}$ | −177.44 (8) |
| Mo3$^{i}$—O6—Mo1—O8 | 98.6 (3) | Mo3$^{i}$—O4—Mo4—O5 | −93.79 (8) |
| Mo4$^{i}$—O6—Mo1—O8 | 14.51 (6) | Mo2—O4—Mo4—O5 | 23.87 (7) |
| Mo2—O6—Mo1—O8 | 178.97 (7) | Mo3$^{i}$—O4—Mo4—O6$^{i}$ | −14.99 (7) |
| Mo3—O6—Mo1—O8 | −83.79 (7) | Mo2—O4—Mo4—O6$^{i}$ | 102.67 (7) |
| Mo3$^{i}$—O6—Mo1—O7 | −178.5 (3) | Mo3$^{i}$—O4—Mo4—Mo3 | −58.03 (6) |
| Mo4$^{i}$—O6—Mo1—O7 | 97.43 (6) | Mo2—O4—Mo4—Mo3 | 59.63 (5) |
| Mo2—O6—Mo1—O7 | −98.11 (6) | O1—Mo3—Mo4—O3 | −108.60 (12) |
| Mo3—O6—Mo1—O7 | −0.87 (5) | O7—Mo3—Mo4—O3 | 3.54 (13) |
| Mo1—O13—Mo2—O12 | 178.35 (10) | O4$^{i}$—Mo3—Mo4—O3 | 147.77 (11) |
| Mo1—O13—Mo2—O11 | 71.32 (11) | O5—Mo3—Mo4—O3 | 1.39 (12) |
| Mo1—O13—Mo2—O4 | −51.82 (18) | O6$^{i}$—Mo3—Mo4—O3 | 149.20 (12) |
| Mo1—O13—Mo2—O6 | −20.65 (9) | O6—Mo3—Mo4—O3 | 76.30 (11) |
| Mo1—O13—Mo2—O5 | −93.66 (10) | Mo2$^{i}$—Mo3—Mo4—O3 | 161.48 (10) |
| Mo1—O13—Mo2—Mo3$^{i}$ | −19.76 (12) | O1—Mo3—Mo4—O2 | 0.31 (9) |
| Mo3$^{i}$—O4—Mo2—O12 | −176.50 (8) | O7—Mo3—Mo4—O2 | 112.46 (10) |
| Mo4—O4—Mo2—O12 | 65.77 (8) | O4$^{i}$—Mo3—Mo4—O2 | −103.32 (9) |
| Mo3$^{i}$—O4—Mo2—O11 | −69.94 (9) | O5—Mo3—Mo4—O2 | 110.30 (11) |
| Mo4—O4—Mo2—O11 | 172.33 (8) | O6$^{i}$—Mo3—Mo4—O2 | −101.89 (9) |
| Mo3$^{i}$—O4—Mo2—O13 | 53.69 (16) | O6—Mo3—Mo4—O2 | −174.78 (8) |
| Mo4—O4—Mo2—O13 | −64.03 (14) | Mo2$^{i}$—Mo3—Mo4—O2 | −89.60 (7) |
| Mo3$^{i}$—O4—Mo2—O6 | 21.81 (7) | O1—Mo3—Mo4—O8$^{i}$ | 101.11 (9) |
| Mo4—O4—Mo2—O6 | −95.92 (7) | O7—Mo3—Mo4—O8$^{i}$ | −146.74 (10) |
| Mo3$^{i}$—O4—Mo2—O5 | 97.78 (8) | O4$^{i}$—Mo3—Mo4—O8$^{i}$ | −2.52 (9) |
| Mo4—O4—Mo2—O5 | −19.95 (5) | O5—Mo3—Mo4—O8$^{i}$ | −148.90 (10) |
| Mo4—O4—Mo2—Mo3$^{i}$ | −117.73 (10) | O6$^{i}$—Mo3—Mo4—O8$^{i}$ | −1.09 (8) |
| Mo3$^{i}$—O6—Mo2—O12 | −93.0 (2) | O6—Mo3—Mo4—O8$^{i}$ | −73.98 (7) |
| Mo4$^{i}$—O6—Mo2—O12 | 164.5 (2) | Mo2$^{i}$—Mo3—Mo4—O8$^{i}$ | 11.20 (6) |
| Mo3—O6—Mo2—O12 | 12.4 (2) | O1—Mo3—Mo4—O5 | −109.99 (10) |
| Mo1—O6—Mo2—O12 | 102.0 (2) | O7—Mo3—Mo4—O5 | 2.15 (11) |
| Mo3$^{i}$—O6—Mo2—O11 | 79.11 (8) | O4$^{i}$—Mo3—Mo4—O5 | 146.38 (10) |
| Mo4$^{i}$—O6—Mo2—O11 | −23.4 (3) | O6$^{i}$—Mo3—Mo4—O5 | 147.81 (10) |
| Mo3—O6—Mo2—O11 | −175.48 (7) | O6—Mo3—Mo4—O5 | 74.92 (9) |
| Mo1—O6—Mo2—O11 | −85.89 (7) | Mo2$^{i}$—Mo3—Mo4—O5 | 160.09 (8) |
| Mo3$^{i}$—O6—Mo2—O13 | 178.84 (7) | O1—Mo3—Mo4—O6$^{i}$ | 102.20 (9) |
| Mo4$^{i}$—O6—Mo2—O13 | 76.4 (3) | O7—Mo3—Mo4—O6$^{i}$ | −145.65 (10) |
| Mo3—O6—Mo2—O13 | −75.74 (7) | O4$^{i}$—Mo3—Mo4—O6$^{i}$ | −1.43 (8) |
| Mo1—O6—Mo2—O13 | 13.85 (6) | O5—Mo3—Mo4—O6$^{i}$ | −147.81 (10) |
| Mo3$^{i}$—O6—Mo2—O4 | −18.46 (6) | O6—Mo3—Mo4—O6$^{i}$ | −72.89 (8) |
| Mo4$^{i}$—O6—Mo2—O4 | −120.9 (3) | Mo2$^{i}$—Mo3—Mo4—O6$^{i}$ | 12.29 (6) |

| | | | |
|---|---|---|---|
| Mo3—O6—Mo2—O4 | 86.95 (7) | O1—Mo3—Mo4—O4 | 176.80 (7) |
| Mo1—O6—Mo2—O4 | 176.54 (7) | O7—Mo3—Mo4—O4 | −71.06 (8) |
| Mo3$^{i}$—O6—Mo2—O5 | −94.59 (6) | O4$^{i}$—Mo3—Mo4—O4 | 73.17 (8) |
| Mo4$^{i}$—O6—Mo2—O5 | 162.9 (3) | O5—Mo3—Mo4—O4 | −73.21 (9) |
| Mo3—O6—Mo2—O5 | 10.83 (5) | O6$^{i}$—Mo3—Mo4—O4 | 74.60 (7) |
| Mo1—O6—Mo2—O5 | 100.42 (5) | O6—Mo3—Mo4—O4 | 1.70 (5) |
| Mo4$^{i}$—O6—Mo2—Mo3$^{i}$ | −102.5 (3) | Mo2$^{i}$—Mo3—Mo4—O4 | 86.88 (4) |

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

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N5—H5N···O11$^{ii}$ | 0.79 (3) | 2.09 (3) | 2.801 (3) | 150 (3) |
| N6—H6N···O9$^{iii}$ | 0.79 (3) | 2.29 (4) | 2.923 (3) | 138 (3) |

Symmetry codes: (ii) −*x*+3/2, −*y*−1/2, −*z*; (iii) *x*, −*y*, *z*+1/2.

**Fig. 1**

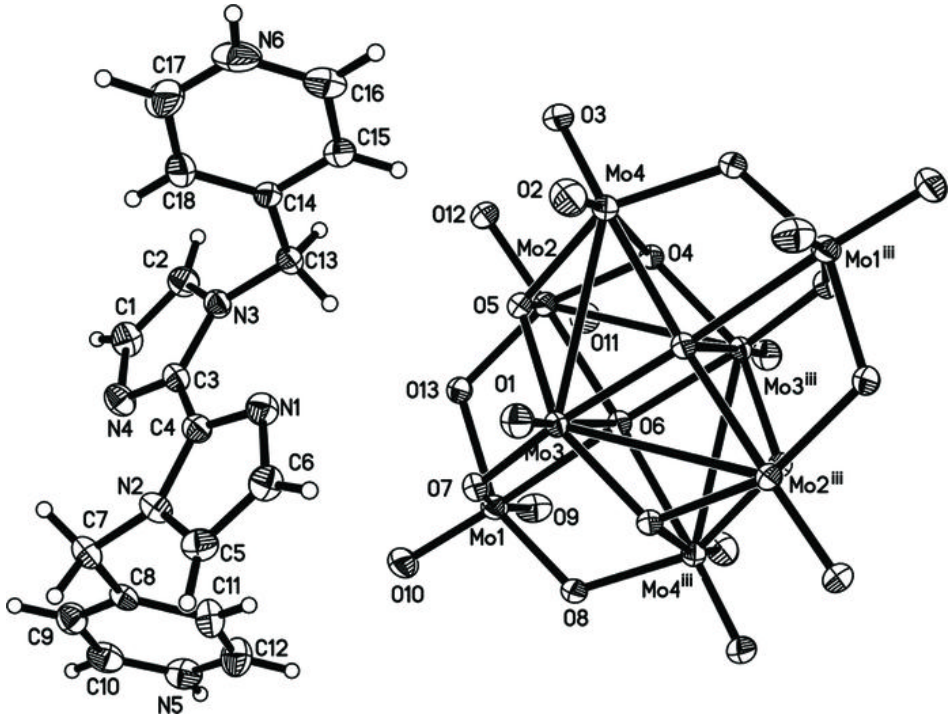
N6
C17
C16
C15
C18
C14
C2
C13
C1
N3
C3
N4
C4
N1
C6
N2
C7
C5
C8
C11
C9
C12
C10
N5
O3
Mo4
O2
O12
Mo2
O4
Mo1iii
O5
O11
O13
O1
Mo3iii
O6
Mo3
Mo2iii
O7
O9
Mo1
O10
O8
Mo4iii

**Fig. 2**