Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis[1,1′-(1,3-phenylenedimethylene)-di(1*H*-imidazol-3-ium)] *β*-octamolybdate

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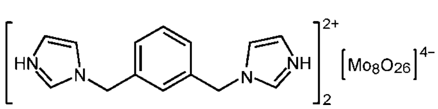
Received 24 November 2011; accepted 9 December 2011

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.026; wR factor = 0.057; data-to-parameter ratio = 16.2.

In the title compound, $(C_{14}H_{16}N_4)_2[Mo_8O_{26}]$, the β-octamolybdate anion is centrosymmetric. N—H···O hydrogen bonds link the diimidazolium cations and the polyoxidoanions into a chain structure along [100]. π–π interactions between the imidazole rings and between the imidazole and benzene rings [centroid–centroid distances = 3.611 (2) and 3.689 (3) Å, respectively] connect the chains.

Related literature

For general background to polyoxidometalate-based organic-inorganic hybrid compounds, see: Xie *et al.* (2011); Xu *et al.* (1999). For the synthesis of the ligand, see: Yang *et al.* (2006).



Experimental

Crystal data

$(C_{14}H_{16}N_4)_2[Mo_8O_{26}]$
M_r = 1664.14
Monoclinic, $P2_1/c$
a = 12.163 (2) Å
b = 12.785 (3) Å
c = 14.937 (3) Å
β = 96.82 (3)°
V = 2306.3 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.20 mm^{-1}
T = 293 K
0.12 × 0.10 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.780, T_{max} = 0.809
21595 measured reflections
5261 independent reflections
4579 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.057
S = 1.01
5261 reflections
324 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 1.12 e Å^{-3}
$\Delta\rho_{min}$ = −1.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H21···O12^{i}	0.90 (1)	1.96 (2)	2.844 (4)	168 (4)
N4—H41···O5^{ii}	0.90 (1)	2.51 (5)	3.003 (5)	115 (4)
N4—H41···O8^{ii}	0.90 (1)	2.23 (4)	2.909 (5)	132 (5)

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

The authors thank the Project of Innovation Service Platform of Heilongjiang Province (PG09J001) and Heilongjiang University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2492).

References

Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Xie, Y.-M., Yu, R.-M., Wu, X.-Y., Wang, F., Zhang, J. & Lu, C.-Z. (2011). *Cryst. Growth Des.* **11**, 4739–4741.
Xu, Q., Wang, R.-Z., Yang, G.-Y., Xing, Y.-H., Li, D.-M., Bu, W.-M., Ye, L., Fan, Y.-G., Yang, G.-D., Xong, Y., Lin, Y.-H. & Jia, H.-Q. (1999). *Chem. Commun.* pp. 983–984.
Yang, J., Ma, J.-F., Liu, Y.-Y., Ma, J.-C., Jia, H.-Q. & Hu, N.-H. (2006). *Eur. J. Inorg. Chem.* pp. 1208–1215.

supplementary materials

Acta Cryst. (2012). E**68**, m50 [**doi:10.1107/S1600536811053050**]

Bis[1,1'-(1,3-phenylenedimethylene)di(1*H*-imidazol-3-ium)] *β*-octamolybdate

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Comment

The synthesis and characterization of coordination networks based on the idea of self-assembly of specifically designed building blocks have been an area of rapid growth in recent years. In the last decades, more and more attention has been paid to the rational design and assembly of new polyoxometalate(POM)-based organic-inorganic hybrid compounds due to their structural diversities and abundant potential applications in catalysis, ion exchange, sorption and magnetism (Xie *et al.*, 2011). Octamolybdate family with a variety of structural isomers is a kind of important POMs building blocks (Xu *et al.*, 1999). The title compound was synthesized at a low pH value condition, as an unexpected product during the process of preparing POM-based Cu(II)–ligand complex. We report its structure here.

The asymmertric unit of the title compound contains one half of β-$[Mo_8O_{26}]^{4-}$ polyoxoanion and one (1,3-phenylenedimethylene)-di-1*H*-imidazolium cation (Fig. 1). The polyoxoanion is centrosymmetric. N—H···O hydrogen bonds link the cations and polyoxoanions into a chain structure along [1 0 0] (Fig. 2, Table 1). *π*–*π* interactions between the imidazole rings and between the imidazole and benzene rings [centroid–centroid distances = 3.611 (2) and 3.689 (3) Å] connect the chains.

Experimental

The 1,3-bis(imidazol-l-yl-methyl)benzene (bimb) ligand was synthesized following the literature method (Yang *et al.*, 2006). The title compound was synthesized by mixing bimb (0.101 g, 0.5 mmol), $Cu(NO_3)_2.4H_2O$ (0.102 g, 0.05 mmol), sodium molybdate (0.505 g, 2.5 mmol), H_2O (8 ml) and ethanol (2 ml) and stirring at room temperature for 10 min. The pH value of the mixture was adjusted to 2.0 with 1M HCl, and then the mixture was sealed in a Teflon-lined autoclave and heated at 125°C for 4 days. After slow cooling to room temperature, black block crystals were obtained in 22% yield based on Mo atoms.

Refinement

The electron density residual peak (1.12) and hole (-1.30) are all around of Mo4 atom with distances of 0.71 and 0.81 Å, respectively. H atoms bound to C atoms were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 (aromatic) and 0.97 (methylene) Å and with $U_{iso}(H) = 1.2U_{eq}(C)$. H atoms bound to N atoms were located from a difference Fourier map and refined isotropically.

Figures

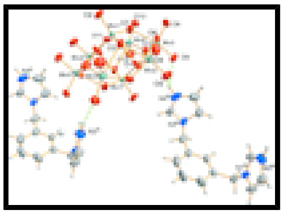

Fig. 1. The molecular structure of the title compound, showing displacement ellipsoids at the 50% probability level. Dashed lines denote hydrogen bonds. [Symmetry codes: (i) 1-x, 2-y, 2-z; (ii) x, 1+y, z; (iii) -1+x, 1+y, z.]

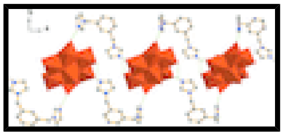

Fig. 2. A view of the hydrogen-bonded chain structure along [1 0 0]. Dashed lines denote hydrogen bonds.

Bis[1,1'-(1,3-phenylenedimethylene)di(1*H*-imidazol-3-ium)] β-octamolybdate

Crystal data

$(C_{14}H_{16}N_4)_2[Mo_8O_{26}]$	$F(000) = 1600$
$M_r = 1664.14$	$D_x = 2.396$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 17887 reflections
$a = 12.163$ (2) Å	$\theta = 3.1$–$27.5°$
$b = 12.785$ (3) Å	$\mu = 2.20$ mm^{-1}
$c = 14.937$ (3) Å	$T = 293$ K
$\beta = 96.82$ (3)°	Block, colorless
$V = 2306.3$ (8) Å^3	0.12 × 0.10 × 0.10 mm
$Z = 2$	

Data collection

Rigaku R-AXIS RAPID diffractometer	5261 independent reflections
Radiation source: fine-focus sealed tube	4579 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.032$
ω scan	$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$h = -15 \rightarrow 15$
$T_{min} = 0.780$, $T_{max} = 0.809$	$k = -16 \rightarrow 15$
21595 measured reflections	$l = -19 \rightarrow 19$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.026$	Hydrogen site location: inferred from neighbouring sites

$wR(F^2) = 0.057$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.01$	$w = 1/[\sigma^2(F_o^2) + (0.0219P)^2 + 3.6973P]$ where $P = (F_o^2 + 2F_c^2)/3$
5261 reflections	$(\Delta/\sigma)_{max} = 0.003$
324 parameters	$\Delta\rho_{max} = 1.12$ e Å^{-3}
2 restraints	$\Delta\rho_{min} = -1.30$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
C1	0.6205 (3)	0.5883 (3)	1.0719 (2)	0.0442 (9)
H1	0.6032	0.6216	1.1237	0.053*
C2	0.6426 (3)	0.6343 (3)	0.9957 (2)	0.0411 (8)
H2	0.6443	0.7059	0.9850	0.049*
C3	0.6529 (3)	0.4656 (3)	0.9766 (3)	0.0414 (8)
H3	0.6623	0.4003	0.9512	0.050*
C4	0.6943 (3)	0.5749 (3)	0.8462 (2)	0.0375 (8)
H4A	0.6747	0.6456	0.8269	0.045*
H4B	0.6542	0.5268	0.8039	0.045*
C5	0.8175 (3)	0.5588 (3)	0.8459 (2)	0.0334 (7)
C6	0.8932 (4)	0.6252 (3)	0.8933 (3)	0.0574 (11)
H6	0.8687	0.6820	0.9245	0.069*
C7	1.0057 (4)	0.6069 (4)	0.8944 (4)	0.0722 (15)
H7	1.0564	0.6506	0.9275	0.087*
C8	1.0431 (3)	0.5248 (4)	0.8469 (4)	0.0638 (13)
H8	1.1188	0.5140	0.8473	0.077*
C9	0.9687 (3)	0.4581 (3)	0.7984 (3)	0.0416 (9)
C10	0.8560 (3)	0.4767 (3)	0.7982 (2)	0.0332 (7)
H10	0.8054	0.4328	0.7652	0.040*
C11	1.0073 (3)	0.3659 (3)	0.7484 (3)	0.0517 (11)
H11A	0.9529	0.3499	0.6974	0.062*
H11B	1.0764	0.3833	0.7254	0.062*
C12	0.9427 (4)	0.2172 (4)	0.8436 (4)	0.0673 (14)
H12	0.8670	0.2300	0.8342	0.081*
C13	0.9922 (5)	0.1420 (4)	0.8937 (4)	0.0722 (15)
H13	0.9581	0.0920	0.9264	0.087*
C14	1.1198 (3)	0.2305 (3)	0.8354 (3)	0.0503 (10)
H14	1.1882	0.2521	0.8202	0.060*
Mo1	0.547848 (19)	0.90288 (2)	1.084672 (17)	0.02207 (6)
Mo2	0.30667 (2)	1.04699 (2)	1.134611 (18)	0.02643 (7)
Mo3	0.27124 (2)	0.86907 (2)	0.973110 (19)	0.02576 (7)
Mo4	0.45286 (2)	0.80953 (3)	0.81444 (2)	0.03626 (8)
N1	0.6622 (2)	0.5573 (2)	0.93667 (18)	0.0312 (6)
N2	0.6281 (3)	0.4835 (3)	1.0589 (2)	0.0463 (8)
N3	1.0240 (2)	0.2736 (3)	0.8073 (2)	0.0425 (7)
N4	1.1028 (4)	0.1517 (3)	0.8884 (3)	0.0622 (10)
O1	0.6277 (2)	0.9749 (2)	1.01029 (18)	0.0472 (7)

O2	0.6373 (2)	0.8237 (2)	1.14858 (18)	0.0477 (7)
O3	0.48333 (18)	0.9874 (2)	1.15775 (16)	0.0372 (6)
O4	0.2810 (2)	1.0400 (2)	1.24323 (16)	0.0439 (6)
O5	0.1925 (2)	1.1056 (2)	1.08042 (19)	0.0500 (7)
O6	0.27884 (17)	0.90605 (17)	1.09648 (15)	0.0298 (5)
O7	0.45232 (19)	0.82404 (19)	1.01803 (19)	0.0429 (6)
O8	0.1530 (2)	0.9344 (2)	0.93423 (17)	0.0417 (6)
O9	0.2328 (2)	0.7420 (2)	0.97568 (19)	0.0439 (6)
O10	0.33456 (19)	0.8728 (2)	0.85883 (16)	0.0361 (5)
O11	0.6000 (2)	0.82712 (18)	0.86168 (17)	0.0371 (5)
O12	0.4326 (2)	0.6786 (2)	0.8263 (2)	0.0548 (7)
O13	0.4385 (3)	0.8367 (2)	0.70317 (19)	0.0555 (7)
H21	0.619 (4)	0.433 (3)	1.099 (2)	0.066 (14)*
H41	1.155 (3)	0.107 (4)	0.911 (4)	0.10 (2)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.052 (2)	0.054 (2)	0.0275 (18)	0.0126 (18)	0.0089 (15)	0.0002 (17)
C2	0.058 (2)	0.0311 (18)	0.035 (2)	0.0116 (16)	0.0088 (16)	−0.0002 (15)
C3	0.051 (2)	0.0339 (19)	0.039 (2)	0.0056 (16)	0.0056 (16)	0.0060 (15)
C4	0.0397 (19)	0.046 (2)	0.0268 (17)	0.0124 (15)	0.0046 (14)	0.0046 (15)
C5	0.0370 (18)	0.0339 (18)	0.0295 (17)	0.0007 (14)	0.0049 (13)	0.0056 (14)
C6	0.062 (3)	0.047 (2)	0.064 (3)	−0.013 (2)	0.012 (2)	−0.013 (2)
C7	0.048 (3)	0.074 (3)	0.093 (4)	−0.028 (2)	0.001 (2)	−0.012 (3)
C8	0.031 (2)	0.082 (4)	0.079 (3)	−0.004 (2)	0.010 (2)	0.010 (3)
C9	0.0353 (19)	0.052 (2)	0.039 (2)	0.0081 (16)	0.0115 (15)	0.0141 (17)
C10	0.0288 (16)	0.043 (2)	0.0277 (17)	0.0024 (14)	0.0033 (12)	0.0024 (14)
C11	0.049 (2)	0.063 (3)	0.047 (2)	0.022 (2)	0.0226 (18)	0.016 (2)
C12	0.044 (2)	0.076 (3)	0.087 (4)	0.012 (2)	0.025 (2)	0.026 (3)
C13	0.085 (4)	0.059 (3)	0.081 (4)	0.021 (3)	0.044 (3)	0.024 (3)
C14	0.038 (2)	0.056 (3)	0.057 (3)	0.0151 (18)	0.0060 (18)	0.006 (2)
Mo1	0.02070 (12)	0.02499 (13)	0.02034 (12)	0.00065 (9)	0.00169 (9)	0.00309 (10)
Mo2	0.02634 (13)	0.03154 (14)	0.02250 (13)	0.00129 (10)	0.00740 (10)	−0.00118 (11)
Mo3	0.02085 (12)	0.02662 (13)	0.03005 (15)	−0.00019 (10)	0.00399 (10)	−0.00093 (11)
Mo4	0.03172 (15)	0.04101 (17)	0.03793 (17)	0.01049 (12)	0.01196 (12)	0.01119 (13)
N1	0.0332 (14)	0.0329 (15)	0.0278 (14)	0.0086 (11)	0.0043 (11)	0.0027 (11)
N2	0.0480 (19)	0.052 (2)	0.0386 (18)	−0.0027 (15)	0.0048 (14)	0.0181 (15)
N3	0.0321 (15)	0.0544 (19)	0.0423 (18)	0.0143 (14)	0.0101 (13)	0.0102 (15)
N4	0.072 (3)	0.057 (2)	0.057 (2)	0.030 (2)	0.005 (2)	0.0138 (19)
O1	0.0685 (18)	0.0394 (14)	0.0395 (15)	−0.0240 (13)	0.0304 (13)	−0.0137 (11)
O2	0.0417 (14)	0.0540 (17)	0.0440 (16)	0.0217 (12)	−0.0092 (11)	0.0005 (13)
O3	0.0266 (12)	0.0462 (14)	0.0375 (14)	0.0049 (10)	−0.0015 (9)	−0.0123 (11)
O4	0.0429 (14)	0.0641 (18)	0.0268 (13)	−0.0067 (12)	0.0124 (10)	−0.0035 (12)
O5	0.0521 (16)	0.0485 (16)	0.0464 (16)	0.0204 (13)	−0.0062 (12)	−0.0066 (13)
O6	0.0279 (11)	0.0316 (12)	0.0299 (12)	−0.0047 (9)	0.0038 (9)	0.0041 (9)
O7	0.0268 (12)	0.0363 (14)	0.0635 (18)	0.0056 (10)	−0.0038 (11)	−0.0175 (12)
O8	0.0347 (13)	0.0524 (16)	0.0370 (14)	0.0147 (11)	−0.0001 (10)	−0.0028 (12)

O9	0.0382 (13)	0.0332 (13)	0.0588 (17)	−0.0100 (10)	−0.0004 (12)	−0.0036 (12)
O10	0.0316 (12)	0.0479 (15)	0.0290 (12)	0.0017 (10)	0.0045 (9)	−0.0064 (11)
O11	0.0449 (14)	0.0251 (11)	0.0435 (15)	0.0036 (10)	0.0149 (11)	−0.0008 (10)
O12	0.0512 (16)	0.0449 (16)	0.070 (2)	−0.0018 (13)	0.0158 (14)	0.0089 (14)
O13	0.073 (2)	0.0581 (18)	0.0390 (16)	0.0120 (15)	0.0235 (14)	0.0048 (14)

Geometric parameters (Å, °)

C1—C2	1.336 (5)	C13—H13	0.9300
C1—N2	1.359 (5)	C14—N3	1.312 (5)
C1—H1	0.9300	C14—N4	1.313 (6)
C2—N1	1.362 (4)	C14—H14	0.9300
C2—H2	0.9300	Mo1—O2	1.695 (2)
C3—N2	1.319 (5)	Mo1—O7	1.756 (2)
C3—N1	1.326 (4)	Mo1—O3	1.783 (2)
C3—H3	0.9300	Mo1—O1	1.811 (2)
C4—N1	1.468 (4)	Mo2—O4	1.690 (2)
C4—C5	1.513 (5)	Mo2—O5	1.697 (3)
C4—H4A	0.9700	Mo2—O6	1.908 (2)
C4—H4B	0.9700	Mo2—O11^{i}	1.966 (2)
C5—C10	1.381 (5)	Mo2—O3	2.267 (2)
C5—C6	1.384 (5)	Mo2—O1^{i}	2.410 (3)
C6—C7	1.387 (7)	Mo3—O9	1.692 (2)
C6—H6	0.9300	Mo3—O8	1.704 (2)
C7—C8	1.374 (7)	Mo3—O6	1.894 (2)
C7—H7	0.9300	Mo3—O10	1.955 (2)
C8—C9	1.383 (6)	Mo3—O7	2.298 (2)
C8—H8	0.9300	Mo3—O1^{i}	2.341 (2)
C9—C10	1.391 (5)	Mo4—O13	1.687 (3)
C9—C11	1.501 (6)	Mo4—O12	1.704 (3)
C10—H10	0.9300	Mo4—O10	1.842 (2)
C11—N3	1.472 (5)	Mo4—O11	1.858 (3)
C11—H11A	0.9700	N2—H21	0.901 (10)
C11—H11B	0.9700	N4—H41	0.896 (10)
C12—C13	1.320 (7)	O1—Mo3^{i}	2.341 (2)
C12—N3	1.385 (5)	O1—Mo2^{i}	2.410 (2)
C12—H12	0.9300	O11—Mo2^{i}	1.966 (2)
C13—N4	1.364 (7)		
C2—C1—N2	106.7 (3)	O4—Mo2—O6	100.96 (12)
C2—C1—H1	126.6	O5—Mo2—O6	99.70 (12)
N2—C1—H1	126.6	O4—Mo2—O11^{i}	100.83 (12)
C1—C2—N1	107.6 (3)	O5—Mo2—O11^{i}	95.11 (13)
C1—C2—H2	126.2	O6—Mo2—O11^{i}	149.63 (10)
N1—C2—H2	126.2	O4—Mo2—O3	96.62 (11)
N2—C3—N1	107.9 (3)	O5—Mo2—O3	158.19 (12)
N2—C3—H3	126.1	O6—Mo2—O3	81.93 (9)
N1—C3—H3	126.1	O11^{i}—Mo2—O3	74.76 (10)

N1—C4—C5	110.7 (3)		O4—Mo2—O1^{i}	166.93 (12)
N1—C4—H4A	109.5		O5—Mo2—O1^{i}	87.85 (12)
C5—C4—H4A	109.5		O6—Mo2—O1^{i}	71.84 (9)
N1—C4—H4B	109.5		O11^{i}—Mo2—O1^{i}	82.45 (9)
C5—C4—H4B	109.5		O3—Mo2—O1^{i}	71.88 (10)
H4A—C4—H4B	108.1		O9—Mo3—O8	104.73 (13)
C10—C5—C6	119.0 (4)		O9—Mo3—O6	101.50 (12)
C10—C5—C4	120.1 (3)		O8—Mo3—O6	98.69 (11)
C6—C5—C4	121.0 (3)		O9—Mo3—O10	100.47 (12)
C5—C6—C7	119.9 (4)		O8—Mo3—O10	95.41 (11)
C5—C6—H6	120.1		O6—Mo3—O10	149.84 (10)
C7—C6—H6	120.1		O9—Mo3—O7	90.60 (11)
C8—C7—C6	120.6 (4)		O8—Mo3—O7	164.34 (12)
C8—C7—H7	119.7		O6—Mo3—O7	81.03 (10)
C6—C7—H7	119.7		O10—Mo3—O7	78.34 (10)
C7—C8—C9	120.3 (4)		O9—Mo3—O1^{i}	163.48 (12)
C7—C8—H8	119.8		O8—Mo3—O1^{i}	91.69 (12)
C9—C8—H8	119.8		O6—Mo3—O1^{i}	73.73 (9)
C8—C9—C10	118.6 (4)		O10—Mo3—O1^{i}	79.36 (10)
C8—C9—C11	121.4 (4)		O7—Mo3—O1^{i}	73.12 (10)
C10—C9—C11	120.0 (4)		O13—Mo4—O12	107.75 (16)
C5—C10—C9	121.5 (3)		O13—Mo4—O10	105.68 (13)
C5—C10—H10	119.2		O12—Mo4—O10	105.41 (13)
C9—C10—H10	119.2		O13—Mo4—O11	109.38 (14)
N3—C11—C9	111.1 (3)		O12—Mo4—O11	102.95 (12)
N3—C11—H11A	109.4		O10—Mo4—O11	124.66 (10)
C9—C11—H11A	109.4		C3—N1—C2	108.4 (3)
N3—C11—H11B	109.4		C3—N1—C4	126.6 (3)
C9—C11—H11B	109.4		C2—N1—C4	124.9 (3)
H11A—C11—H11B	108.0		C3—N2—C1	109.3 (3)
C13—C12—N3	107.7 (4)		C3—N2—H21	124 (3)
C13—C12—H12	126.2		C1—N2—H21	127 (3)
N3—C12—H12	126.2		C14—N3—C12	107.7 (4)
C12—C13—N4	106.7 (4)		C14—N3—C11	125.6 (3)
C12—C13—H13	126.7		C12—N3—C11	126.7 (3)
N4—C13—H13	126.7		C14—N4—C13	109.4 (4)
N3—C14—N4	108.6 (4)		C14—N4—H41	125 (4)
N3—C14—H14	125.7		C13—N4—H41	125 (4)
N4—C14—H14	125.7		Mo1—O1—Mo3^{i}	132.92 (13)
O2—Mo1—O7	108.29 (13)		Mo1—O1—Mo2^{i}	138.66 (13)
O2—Mo1—O3	108.47 (12)		Mo3^{i}—O1—Mo2^{i}	88.18 (8)
O7—Mo1—O3	112.67 (11)		Mo1—O3—Mo2	126.04 (12)
O2—Mo1—O1	107.09 (14)		Mo3—O6—Mo2	120.84 (11)
O7—Mo1—O1	108.11 (13)		Mo1—O7—Mo3	124.65 (12)
O3—Mo1—O1	111.99 (12)		Mo4—O10—Mo3	135.18 (14)
O4—Mo2—O5	104.33 (14)		Mo4—O11—Mo2^{i}	129.54 (13)

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

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H21···O12^{ii}	0.90 (1)	1.96 (2)	2.844 (4)	168 (4)
N4—H41···O5^{iii}	0.90 (1)	2.51 (5)	3.003 (5)	115 (4)
N4—H41···O8^{iii}	0.90 (1)	2.23 (4)	2.909 (5)	132 (5)

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

Fig. 1

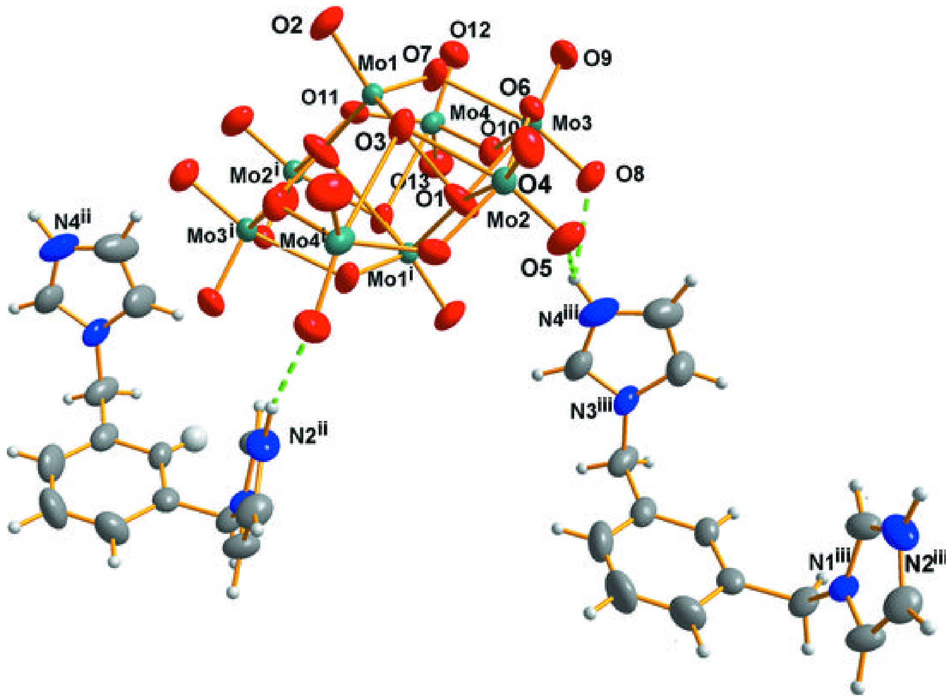
O2
O12
Mo1
O7
O9
O11
O6
Mo4
O10
Mo3
O3
Mo2i
O13
O1
O4
O8
Mo2
Mo3i
Mo4i
Mo1i
O5
N4ii
N4iii
N3iii
N2ii
N1iii
N2iii

Fig. 2