

## Tetraimidazolium hexa- $\mu_4$ -oxido-dodeca- $\mu_2$ -oxido-dodecaoxidohexaarsenate(III)-hexamolybdenum(VI)cuprate(II)

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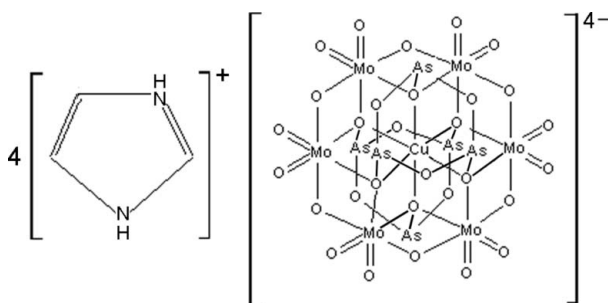
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.009$  Å;  $R$  factor = 0.030;  $wR$  factor = 0.073; data-to-parameter ratio = 17.2.

The title compound,  $(\text{C}_3\text{H}_5\text{N}_2)_4[\text{As}_6\text{CuMo}_6\text{O}_{30}]$ , is made up of a centrosymmetric anionic cluster and four imidazolium cations. In the cluster, the central  $\text{Cu}^{\text{II}}$  atom is six-coordinated and lies on an inversion center. Adjacent clusters are linked *via*  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds between the imidazole cations and polyoxidoanions into a three-dimensional supramolecular architecture.

### Related literature

For general background to polyoxido-metalates, see: Müller *et al.* (1998). For general background to molybdoarsenates, see: Fidalgo *et al.* (2002); Sun *et al.* (2007).



### Experimental

#### Crystal data

$(\text{C}_3\text{H}_5\text{N}_2)_4[\text{As}_6\text{CuMo}_6\text{O}_{30}]$   
 $M_r = 1845.07$   
 Monoclinic,  $P2_1/c$   
 $a = 10.5696$  (7) Å  
 $b = 19.2842$  (12) Å  
 $c = 10.4678$  (7) Å  
 $\beta = 106.747$  (1)°

$V = 2043.1$  (2) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 7.22$  mm<sup>-1</sup>  
 $T = 298$  K  
 $0.28 \times 0.25 \times 0.20$  mm

#### Data collection

Bruker APEXII CCD diffractometer  
 Absorption correction: multi-scan (*SADABS*; Bruker, 2001)  
 $T_{\text{min}} = 0.237$ ,  $T_{\text{max}} = 0.326$

12666 measured reflections  
 4906 independent reflections  
 4057 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.029$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.030$   
 $wR(F^2) = 0.073$   
 $S = 1.03$   
 4906 reflections  
 286 parameters

1 restraint  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.56$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -1.94$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1A}\cdots\text{O4}^{\text{i}}$	0.86	1.81	2.664 (5)	173
$\text{N2}-\text{H2A}\cdots\text{O3}$	0.86	1.99	2.748 (5)	146
$\text{N2}-\text{H2A}\cdots\text{O9}^{\text{ii}}$	0.86	2.42	3.020 (5)	127
$\text{N3}-\text{H3A}\cdots\text{O7}^{\text{ii}}$	0.86	2.09	2.867 (6)	150
$\text{N4}-\text{H4A}\cdots\text{O2}^{\text{iii}}$	0.86	2.00	2.834 (6)	165

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: HY2352).

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**supplementary materials**

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**Tetraimidazolium  
dodecaoxidohexaarsenate(III)hexamolybdenum(VI)cuprate(II)**

**hexa- $\mu_4$ -oxido-dodeca- $\mu_2$ -oxido-**

**M. Liu, Z. Su and Y. Shang**

**Comment**

Polyoxometalates have unusual structural chemistry and properties that make them attractive for applications in materials science, electrochemical, catalysis and photochemical (Müller *et al.*, 1998). Molybdenum arsenates are an important part in this field. So far the reports on molybdenum arsenates have been mainly concentrated on several discrete molybdenum arsenate clusters (Fidalgo *et al.*, 2002; Sun *et al.*, 2007). Therefore, further research is necessary to enrich and develop this branch. We try to obtain new materials based on inorganic molybdenum arsenate with novel structures. Here, the synthesis and crystal structure of the title compound is reported.

The structure of the title compound is shown in Fig. 1. The asymmetric unit consists of two protonated imidazole cations and a half cluster anion. The anion is centrosymmetric with the Cu<sup>II</sup> atom lying on an inversion center. The cluster is derived from the A-type Anderson anion, in which a central CuO<sub>6</sub> octahedron is coordinated with six MoO<sub>6</sub> octahedra hexagonally arranged by sharing their edges in a plane. Two cyclic As<sub>3</sub>O<sub>3</sub> trimers are capped on the opposite faces of the Anderson-type anion plane. The four free protonated imidazole molecules act as charge compensating cations. The adjacent clusters are linked *via* N—H $\cdots$ O hydrogen bonds between the imidazole cations and polyoxoanions into a three-dimensional supramolecular architecture (Table 1).

**Experimental**

A mixture of hexaammonium heptamolybdate tetrahydrate (1.11 g, 0.89 mmol), sodium arsenite (0.41 g, 3.03 mmol), cupric chloride (0.20 g, 1.17 mmol), imidazole (0.27 g, 4.01 mmol) and water (20 ml) was placed in a 30 ml Teflon-lined Parr bomb. The bomb was heated to 413 K for 5 d. Blue block shaped crystals were isolated from the cooled solution in a 72% yield based on Mo. Analysis, calculated for C<sub>12</sub>H<sub>20</sub>As<sub>6</sub>CuMo<sub>6</sub>N<sub>8</sub>O<sub>30</sub>: C 7.81, H 1.09, N 6.07%; found: C 7.83, H 1.13, N 6.04%.

**Refinement**

H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 and N—H = 0.86 Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ .

**Figures**

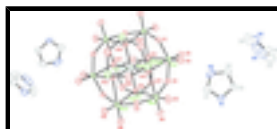


Fig. 1. The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted. [Symmetry code: (i) 2-x, -y, -z.]

## Tetraimidazolium hexa- $\mu_4$ -oxido-dodeca- $\mu_2$ -oxido-dodecaoxidohexaarsenate(III)hexamolybdenum(VI)cuprate(II)

### Crystal data

$(C_3H_5N_2)_4[As_6CuMo_6O_{30}]$	$F(000) = 1734$
$M_r = 1845.07$	$D_x = 2.999 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2ybc	Cell parameters from 4555 reflections
$a = 10.5696 (7) \text{ \AA}$	$\theta = 2.3\text{--}28.1^\circ$
$b = 19.2842 (12) \text{ \AA}$	$\mu = 7.22 \text{ mm}^{-1}$
$c = 10.4678 (7) \text{ \AA}$	$T = 298 \text{ K}$
$\beta = 106.747 (1)^\circ$	Block, blue
$V = 2043.1 (2) \text{ \AA}^3$	$0.28 \times 0.25 \times 0.20 \text{ mm}$
$Z = 2$	

### Data collection

Bruker APEXII CCD diffractometer	4906 independent reflections
Radiation source: fine-focus sealed tube graphite	4057 reflections with $I > 2\sigma(I)$
$\varphi$ and $\omega$ scans	$R_{\text{int}} = 0.029$
Absorption correction: multi-scan ( <i>SADABS</i> ; Bruker, 2001)	$\theta_{\text{max}} = 28.3^\circ$ , $\theta_{\text{min}} = 2.3^\circ$
$T_{\text{min}} = 0.237$ , $T_{\text{max}} = 0.326$	$h = -13 \rightarrow 14$
12666 measured reflections	$k = -25 \rightarrow 19$
	$l = -13 \rightarrow 13$

### Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.030$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.073$	H-atom parameters constrained
$S = 1.03$	$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 2.1525P]$
4906 reflections	where $P = (F_o^2 + 2F_c^2)/3$
286 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
1 restraint	$\Delta\rho_{\text{max}} = 0.56 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -1.94 \text{ e \AA}^{-3}$

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Mo1	0.73132 (3)	0.054936 (18)	0.07751 (3)	0.01939 (9)

Mo2	1.01930 (3)	0.143475 (18)	0.18894 (3)	0.02087 (9)
Mo3	1.29116 (3)	0.084229 (18)	0.11868 (4)	0.02065 (9)
Cu1	1.0000	0.0000	0.0000	0.02300 (16)
As1	1.03800 (5)	0.16004 (2)	-0.13845 (4)	0.02655 (11)
As2	0.75566 (4)	0.08081 (2)	-0.24782 (4)	0.02711 (11)
As3	0.98689 (4)	-0.02215 (2)	0.32318 (4)	0.02600 (11)
O1	0.7044 (3)	-0.04164 (14)	0.0461 (3)	0.0222 (6)
O2	0.5905 (3)	0.09037 (16)	-0.0244 (3)	0.0324 (7)
O3	0.7135 (3)	0.05775 (16)	0.2348 (3)	0.0301 (7)
O4	0.8381 (3)	0.13750 (14)	0.0796 (3)	0.0222 (6)
O5	0.9982 (3)	0.14957 (17)	0.3446 (3)	0.0335 (7)
O6	1.0471 (3)	0.22633 (16)	0.1453 (3)	0.0347 (7)
O7	1.1939 (3)	0.10410 (15)	0.2460 (3)	0.0240 (6)
O8	1.3348 (3)	0.16566 (16)	0.0847 (3)	0.0355 (8)
O9	1.4277 (3)	0.05057 (17)	0.2328 (3)	0.0330 (7)
O10	1.0708 (3)	0.10168 (14)	0.0027 (3)	0.0194 (6)
O11	0.8615 (3)	0.15371 (15)	-0.1931 (3)	0.0311 (7)
O12	0.8071 (3)	0.02681 (14)	-0.1035 (3)	0.0190 (6)
O13	0.9515 (3)	0.02733 (14)	0.1712 (3)	0.0193 (6)
O14	0.9234 (3)	-0.10364 (16)	0.2570 (3)	0.0294 (7)
O15	1.1601 (3)	-0.03719 (17)	0.3501 (3)	0.0306 (7)
C1	0.7300 (6)	0.1970 (3)	0.4181 (6)	0.0547 (16)
H1	0.8100	0.1911	0.3989	0.066*
C2	0.5755 (5)	0.2391 (3)	0.4939 (5)	0.0402 (12)
H2	0.5301	0.2679	0.5369	0.048*
C3	0.5305 (6)	0.1807 (3)	0.4292 (6)	0.0481 (14)
H3	0.4477	0.1610	0.4181	0.058*
C4	0.2581 (6)	0.1681 (3)	0.5787 (6)	0.0498 (14)
H4	0.2056	0.2032	0.5297	0.060*
C5	0.3261 (7)	0.1725 (4)	0.7012 (7)	0.072 (2)
H5	0.3326	0.2109	0.7565	0.087*
C6	0.3535 (7)	0.0703 (4)	0.6296 (9)	0.072 (2)
H6	0.3815	0.0249	0.6254	0.086*
N1	0.6994 (4)	0.2487 (2)	0.4856 (5)	0.0422 (11)
H1A	0.7501	0.2831	0.5190	0.051*
N2	0.6282 (5)	0.1554 (2)	0.3826 (5)	0.0511 (13)
H2A	0.6240	0.1179	0.3369	0.061*
N3	0.2742 (4)	0.1053 (3)	0.5320 (5)	0.0493 (12)
H3A	0.2388	0.0906	0.4521	0.059*
N4	0.3864 (5)	0.1108 (5)	0.7346 (6)	0.091 (3)
H4A	0.4378	0.0998	0.8118	0.109*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Mo1	0.01533 (17)	0.02100 (17)	0.02186 (18)	0.00083 (13)	0.00538 (13)	-0.00261 (13)
Mo2	0.01802 (18)	0.02131 (18)	0.02259 (18)	-0.00029 (14)	0.00474 (14)	-0.00575 (13)
Mo3	0.01496 (17)	0.02128 (18)	0.02509 (19)	-0.00293 (13)	0.00477 (14)	-0.00520 (13)

## supplementary materials

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Cu1	0.0210 (4)	0.0247 (4)	0.0227 (4)	-0.0005 (3)	0.0052 (3)	-0.0014 (3)
As1	0.0304 (3)	0.0220 (2)	0.0268 (2)	-0.00166 (18)	0.00755 (19)	0.00428 (17)
As2	0.0213 (2)	0.0327 (2)	0.0245 (2)	0.00458 (18)	0.00205 (18)	0.00643 (18)
As3	0.0291 (2)	0.0318 (2)	0.0175 (2)	0.00211 (19)	0.00728 (18)	0.00140 (17)
O1	0.0210 (15)	0.0219 (14)	0.0254 (15)	-0.0049 (12)	0.0095 (12)	-0.0016 (11)
O2	0.0228 (16)	0.0330 (18)	0.0384 (18)	0.0045 (13)	0.0038 (14)	-0.0019 (14)
O3	0.0300 (17)	0.0327 (17)	0.0309 (17)	-0.0025 (14)	0.0142 (14)	-0.0056 (13)
O4	0.0188 (14)	0.0185 (14)	0.0270 (15)	0.0012 (11)	0.0029 (12)	-0.0012 (11)
O5	0.0263 (17)	0.046 (2)	0.0284 (17)	0.0003 (14)	0.0087 (14)	-0.0085 (14)
O6	0.0355 (18)	0.0233 (16)	0.045 (2)	-0.0010 (14)	0.0103 (15)	-0.0075 (14)
O7	0.0185 (14)	0.0308 (16)	0.0209 (14)	-0.0014 (12)	0.0028 (11)	-0.0075 (12)
O8	0.0338 (18)	0.0262 (16)	0.050 (2)	-0.0092 (14)	0.0182 (16)	-0.0082 (15)
O9	0.0175 (15)	0.0403 (19)	0.0362 (18)	0.0017 (14)	-0.0005 (13)	-0.0076 (14)
O10	0.0177 (14)	0.0203 (14)	0.0196 (14)	-0.0009 (11)	0.0046 (11)	-0.0005 (11)
O11	0.0302 (17)	0.0274 (16)	0.0338 (18)	0.0048 (13)	0.0063 (14)	0.0065 (13)
O12	0.0150 (13)	0.0215 (14)	0.0190 (14)	-0.0002 (11)	0.0028 (11)	0.0025 (11)
O13	0.0185 (14)	0.0213 (14)	0.0178 (13)	0.0018 (11)	0.0049 (11)	0.0000 (11)
O14	0.0324 (17)	0.0286 (16)	0.0296 (17)	-0.0015 (13)	0.0126 (14)	0.0037 (13)
O15	0.0294 (17)	0.0382 (18)	0.0213 (15)	0.0017 (14)	0.0028 (13)	0.0038 (13)
C1	0.052 (4)	0.047 (3)	0.076 (4)	-0.002 (3)	0.036 (3)	-0.008 (3)
C2	0.038 (3)	0.036 (3)	0.050 (3)	0.000 (2)	0.017 (2)	-0.010 (2)
C3	0.048 (3)	0.048 (3)	0.053 (3)	-0.021 (3)	0.021 (3)	-0.017 (3)
C4	0.052 (4)	0.044 (3)	0.048 (3)	0.011 (3)	0.005 (3)	0.010 (3)
C5	0.073 (5)	0.084 (5)	0.059 (4)	-0.036 (4)	0.018 (4)	-0.023 (4)
C6	0.062 (5)	0.054 (4)	0.112 (7)	0.019 (3)	0.045 (5)	0.049 (4)
N1	0.037 (2)	0.028 (2)	0.061 (3)	-0.0103 (18)	0.014 (2)	-0.0152 (19)
N2	0.074 (4)	0.032 (2)	0.057 (3)	-0.012 (2)	0.034 (3)	-0.019 (2)
N3	0.038 (3)	0.055 (3)	0.048 (3)	-0.009 (2)	0.000 (2)	-0.004 (2)
N4	0.034 (3)	0.190 (8)	0.041 (3)	0.001 (4)	0.000 (3)	0.060 (4)

### *Geometric parameters (Å, °)*

Mo1—O2	1.704 (3)	As2—O11	1.785 (3)
Mo1—O3	1.711 (3)	As2—O12	1.786 (3)
Mo1—O1	1.898 (3)	As2—O15 <sup>i</sup>	1.788 (3)
Mo1—O4	1.948 (3)	As3—O14	1.770 (3)
Mo1—O13	2.312 (3)	As3—O15	1.793 (3)
Mo1—O12	2.324 (3)	As3—O13	1.800 (3)
Mo2—O6	1.710 (3)	C1—N2	1.308 (7)
Mo2—O5	1.711 (3)	C1—N1	1.316 (7)
Mo2—O7	1.925 (3)	C1—H1	0.9300
Mo2—O4	1.931 (3)	C2—C3	1.329 (7)
Mo2—O10	2.315 (3)	C2—N1	1.351 (6)
Mo2—O13	2.343 (3)	C2—H2	0.9300
Mo3—O8	1.703 (3)	C3—N2	1.354 (7)
Mo3—O9	1.714 (3)	C3—H3	0.9300
Mo3—O1 <sup>i</sup>	1.923 (3)	C4—C5	1.280 (9)
Mo3—O7	1.941 (3)	C4—N3	1.334 (7)
Mo3—O10	2.320 (3)	C4—H4	0.9300

Mo3—O12 <sup>i</sup>	2.365 (3)	C5—N4	1.349 (10)
Cu1—O13	2.069 (3)	C5—H5	0.9300
Cu1—O13 <sup>i</sup>	2.069 (3)	C6—N3	1.308 (8)
Cu1—O12	2.080 (3)	C6—N4	1.310 (10)
Cu1—O12 <sup>i</sup>	2.080 (3)	C6—H6	0.9300
Cu1—O10 <sup>i</sup>	2.096 (3)	N1—H1A	0.8600
Cu1—O10	2.096 (3)	N2—H2A	0.8600
As1—O14 <sup>i</sup>	1.783 (3)	N3—H3A	0.8600
As1—O11	1.791 (3)	N4—H4A	0.8600
As1—O10	1.810 (3)		
O2—Mo1—O3	105.76 (15)	O11—As1—O10	98.94 (13)
O2—Mo1—O1	102.98 (14)	O11—As2—O12	100.25 (13)
O3—Mo1—O1	98.34 (13)	O11—As2—O15 <sup>i</sup>	100.87 (15)
O2—Mo1—O4	94.47 (13)	O12—As2—O15 <sup>i</sup>	98.60 (13)
O3—Mo1—O4	100.78 (13)	O14—As3—O15	99.93 (14)
O1—Mo1—O4	149.46 (12)	O14—As3—O13	99.56 (13)
O2—Mo1—O13	161.51 (13)	O15—As3—O13	99.65 (13)
O3—Mo1—O13	88.59 (12)	Mo1—O1—Mo3 <sup>i</sup>	122.20 (14)
O1—Mo1—O13	85.98 (11)	Mo2—O4—Mo1	121.87 (14)
O4—Mo1—O13	70.99 (10)	Mo2—O7—Mo3	121.00 (14)
O2—Mo1—O12	91.53 (13)	As1—O10—Cu1	125.93 (14)
O3—Mo1—O12	162.04 (13)	As1—O10—Mo2	115.77 (13)
O1—Mo1—O12	72.51 (10)	Cu1—O10—Mo2	99.64 (10)
O4—Mo1—O12	82.27 (10)	As1—O10—Mo3	116.41 (13)
O13—Mo1—O12	75.58 (9)	Cu1—O10—Mo3	99.92 (11)
O6—Mo2—O5	105.65 (16)	Mo2—O10—Mo3	93.11 (9)
O6—Mo2—O7	103.19 (14)	As2—O11—As1	130.91 (17)
O5—Mo2—O7	96.23 (14)	As2—O12—Cu1	126.82 (14)
O6—Mo2—O4	96.59 (13)	As2—O12—Mo1	117.47 (13)
O5—Mo2—O4	100.89 (13)	Cu1—O12—Mo1	98.60 (10)
O7—Mo2—O4	149.22 (11)	As2—O12—Mo3 <sup>i</sup>	116.78 (13)
O6—Mo2—O10	90.01 (13)	Cu1—O12—Mo3 <sup>i</sup>	98.95 (10)
O5—Mo2—O10	162.31 (13)	Mo1—O12—Mo3 <sup>i</sup>	91.05 (9)
O7—Mo2—O10	71.73 (10)	As3—O13—Cu1	126.18 (14)
O4—Mo2—O10	85.07 (11)	As3—O13—Mo1	115.12 (13)
O6—Mo2—O13	160.76 (13)	Cu1—O13—Mo1	99.30 (10)
O5—Mo2—O13	91.16 (13)	As3—O13—Mo2	117.13 (13)
O7—Mo2—O13	83.77 (11)	Cu1—O13—Mo2	99.54 (11)
O4—Mo2—O13	70.57 (10)	Mo1—O13—Mo2	93.50 (10)
O10—Mo2—O13	75.00 (9)	As3—O14—As1 <sup>i</sup>	132.63 (17)
O8—Mo3—O9	105.69 (16)	As2 <sup>i</sup> —O15—As3	130.07 (17)
O8—Mo3—O1 <sup>i</sup>	97.38 (14)	N2—C1—N1	108.0 (5)
O9—Mo3—O1 <sup>i</sup>	103.31 (14)	N2—C1—H1	126.0
O8—Mo3—O7	100.96 (14)	N1—C1—H1	126.0
O9—Mo3—O7	95.87 (13)	C3—C2—N1	107.2 (5)

## supplementary materials

O1 <sup>i</sup> —Mo3—O7	148.71 (11)	C3—C2—H2	126.4
O8—Mo3—O10	92.78 (13)	N1—C2—H2	126.4
O9—Mo3—O10	159.45 (13)	C2—C3—N2	107.0 (5)
O1 <sup>i</sup> —Mo3—O10	82.70 (11)	C2—C3—H3	126.5
O7—Mo3—O10	71.35 (10)	N2—C3—H3	126.5
O8—Mo3—O12 <sup>i</sup>	163.96 (13)	C5—C4—N3	109.5 (6)
O9—Mo3—O12 <sup>i</sup>	88.23 (13)	C5—C4—H4	125.2
O1 <sup>i</sup> —Mo3—O12 <sup>i</sup>	71.15 (10)	N3—C4—H4	125.2
O7—Mo3—O12 <sup>i</sup>	85.17 (11)	C4—C5—N4	106.7 (7)
O10—Mo3—O12 <sup>i</sup>	74.99 (9)	C4—C5—H5	126.7
O13—Cu1—O13 <sup>i</sup>	180.0	N4—C5—H5	126.7
O13—Cu1—O12	86.42 (10)	N3—C6—N4	107.7 (6)
O13 <sup>i</sup> —Cu1—O12	93.58 (10)	N3—C6—H6	126.2
O13—Cu1—O12 <sup>i</sup>	93.58 (10)	N4—C6—H6	126.2
O13 <sup>i</sup> —Cu1—O12 <sup>i</sup>	86.42 (10)	C1—N1—C2	108.8 (4)
O12—Cu1—O12 <sup>i</sup>	180.0	C1—N1—H1A	125.6
O13—Cu1—O10 <sup>i</sup>	94.21 (10)	C2—N1—H1A	125.6
O13 <sup>i</sup> —Cu1—O10 <sup>i</sup>	85.79 (10)	C1—N2—C3	109.1 (5)
O12—Cu1—O10 <sup>i</sup>	86.14 (10)	C1—N2—H2A	125.5
O12 <sup>i</sup> —Cu1—O10 <sup>i</sup>	93.86 (10)	C3—N2—H2A	125.5
O13—Cu1—O10	85.79 (10)	C6—N3—C4	107.6 (6)
O13 <sup>i</sup> —Cu1—O10	94.21 (10)	C6—N3—H3A	126.2
O12—Cu1—O10	93.86 (10)	C4—N3—H3A	126.2
O12 <sup>i</sup> —Cu1—O10	86.14 (10)	C6—N4—C5	108.5 (5)
O10 <sup>i</sup> —Cu1—O10	180.0	C6—N4—H4A	125.8
O14 <sup>i</sup> —As1—O11	99.33 (14)	C5—N4—H4A	125.8
O14 <sup>i</sup> —As1—O10	99.24 (13)		

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

### Hydrogen-bond geometry ( $\text{\AA}, ^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1A $\cdots$ O4 <sup>ii</sup>	0.86	1.81	2.664 (5)	173
N2—H2A $\cdots$ O3	0.86	1.99	2.748 (5)	146
N2—H2A $\cdots$ O9 <sup>iii</sup>	0.86	2.42	3.020 (5)	127
N3—H3A $\cdots$ O7 <sup>iii</sup>	0.86	2.09	2.867 (6)	150
N4—H4A $\cdots$ O2 <sup>iv</sup>	0.86	2.00	2.834 (6)	165

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



Fig. 1

