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Bis(amino{[iminio(morpholino)methyl]-amino}iminium) bis(amino{[imino-(morpholino)methyl]amino}iminium) tetracosaoxidotellurohexamolybdate(6−) tetrahydrate

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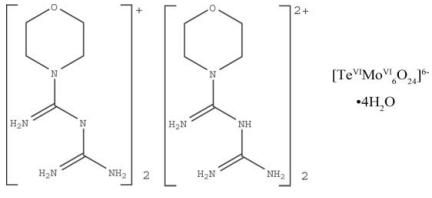
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.025; wR factor = 0.056; data-to-parameter ratio = 13.0.

The title compound, $(H_2ABOB)_2(HABOB)_2[Te^{VI}Mo^{VI}_6O_{24}]\cdot 4H_2O$, consists of an Anderson-type heteropolyanion, $[Te^{VI}Mo^{VI}_6O_{24}]^{6-}$, two monoprotonated ABOB cations, two diprotonated ABOB cations and four water molecules (ABOB = *N*-amidino-4-morpholincarboxamidine). The heteropolyanion $[Te^{VI}Mo^{VI}_6O_{24}]^{6-}$ is located on an inversion center. Electrostatic forces and hydrogen-bonding interactions among the $[Te^{VI}Mo^{VI}_6O_{24}]^{6-}$anions, the water molecules and the ABOB cations result in a three-dimensional supramolecular structure.

Related literature

For similar structures, see: Chen *et al.* (2007); Li *et al.* (2005); Liu *et al.* (2004); Drewes *et al.* (2004); Gao *et al.* (2006). For the synthesis of the $[Te^{VI}Mo^{VI}_6O_{24}]^{6-}$ polyanion, see Saito (1994).



Experimental

Crystal data

$(C_6H_{15}N_5O)_2(C_6H_{14}N_5O)_2[TeMo_6O_{24}].4H_2O$
M_r = 1850.21
Monoclinic, $P2_1/n$
a = 15.722 (3) Å
b = 9.2364 (18) Å
c = 19.256 (4) Å
β = 94.67 (3)°
V = 2787.0 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.93 mm^{-1}
T = 298 (2) K
0.24 × 0.24 × 0.22 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.643, T_{max} = 0.657
20771 measured reflections
4883 independent reflections
4465 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.056
S = 1.09
4883 reflections
377 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.86 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H6···O7	0.90	2.20	2.916 (3)	137
N1—H5···O2	0.90	2.04	2.769 (3)	138
N2—H8···O1^{i}	0.90	1.95	2.840 (3)	172
N2—H7···O1*W*	0.90	2.01	2.877 (3)	162
N3—H9···O10^{ii}	0.90	1.69	2.571 (3)	165
N4—H11···O11^{iii}	0.90	2.18	2.965 (3)	146
N4—H10···O2*W*^{i}	0.90	1.86	2.762 (4)	177
N9—H17···O14^{iv}	0.90	2.18	3.067 (4)	167
N7—H15···O9	0.90	2.14	2.925 (4)	146
N7—H14···O7^{v}	0.90	2.05	2.921 (3)	164
N6—H13···O8^{v}	0.90	2.06	2.806 (4)	140
O1*W*—H1···O3^{vi}	0.85	1.97	2.810 (3)	172
O1*W*—H2···O12	0.85	2.61	3.087 (3)	117
O1*W*—H2···O14^{iv}	0.85	2.25	3.027 (3)	152
O2*W*—H3···O5^{i}	0.85	2.06	2.860 (3)	156
O2*W*—H4···O1*W*	0.85	1.98	2.829 (4)	176

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

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXTL* (Bruker, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2263).

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supplementary materials

Acta Cryst. (2007). E**63**, m1708-m1709 [**doi:10.1107/S1600536807023525**]

Bis(amino{[iminio(morpholino)methyl]amino}iminium) bis(amino{[imino(morpholino)methyl]amino}iminium) tetracosaoxidotellurohexamolybdate(6-) tetrahydrate

F. Wang, S.-X. Liu, C.-L. Wang, R.-G. Cao and J.-F. Cao

Comment

N-Amidino-4-morpholincarboxamidine (ABOB) is an effective broad-spectrum antiviral medicine to influenza, chicken-pox and measles. In our chemical studies (Chen *et al.*, 2007; Li *et al.*, 2005; Liu *et al.*, 2004), we found it is a versatile ligand capable of interacting with different types of polyanions. As a part of our ongoing work, we have investigated the reaction of ABOB and the Anderson type $[Te^{VI}Mo^{VI}_6O_{24}]^{6-}$ polyanion to give a compound formulated as $(H_2ABOB)_2(HABOB)_2[Te^{VI}Mo^{VI}_6O_{24}]\cdot 4H_2O$ (I).

The compound consists of $[Te^{VI}Mo^{VI}_6O_{24}]^{6-}$, protonated ABOB, and lattice water molecules. The three-dimensional supramolecular structure is formed by electrostatic forces and hydrogen bonding interactions among these components (Fig. 1). The $[Te^{VI}Mo^{VI}_6O_{24}]^{6-}$ anion lies on an inversion center and is close to having $D_{3\,d}$ symmetry. It is made up of six MoO_6 octahedra surrounding one TeO_6 octahedron by entirely edge-shared contacts; bond lengths and angles are in accordance with those of reported examples (Drewes *et al.*, 2004; Gao *et al.*, 2006) The diprotonated ABOB acquires two protons with its two imine groups (N2, N4). The monoprotonated ABOB acquires two protons with two imine groups (N6, N9) as well but loses one proton on the third imine groups (N8). Electrostatic forces and hydrogen bonding interactions result in a three-dimensional supramolecular structure (Figure 2, Figure 3). The hydrogen-bond donors are the protonated imines groups and water molecules whereas the acceptors are mostly the O atoms of the Anderson type polyanion.

Experimental

A mixture of $Na_6[Te^{VI}Mo^{VI}_6O_{24}]^{6-}\cdot 22H_2O$ (0.32 g, 0.2 mmol) (Saito, 1994)) and ABOB (0.21 g, 1.2 mmol) in water (30 ml) treated with dilute hydrochloric acid to pH 5–6. The solution was stirred for 2 h. It was then filtered; the filtrate was set aside for the formation of crystals after two weeks; yield 65% based on Te.

Refinement

The H atoms on water molecules, amine, and protonated imine groups were located in a difference Fourier map, and refined with distance restraints of with O–H = 0.85 Å, N–H = 0.90 Å and U_{iso}(H) = 1.2 U_{eq}(O,*N*). Those on C atoms are placed in calculated positions and refined in the riding model approximation with C–H = 0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

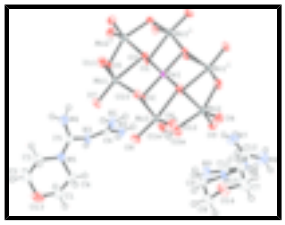

Fig. 1. **Figure 1**. *ORTEP* view of (I) with displacement ellipsoids drawn at 50% probability level. [Symmetry code: (i) $2-x, 2-y, -z$.]

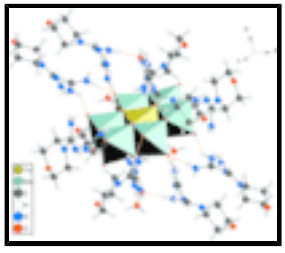

Fig. 2. **Figure 2**. Hydrogen bonds (yellow dotted line) around a polyanion which is represented as polyhedra.

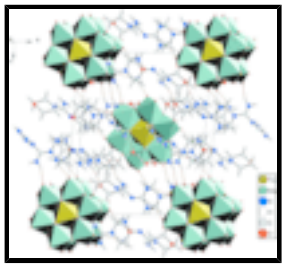

Fig. 3. **Figure 3**. The crystal packing in a unit cell, with hydrogen bonds showed as yellow dotted line and polyanions represented as polyhedra.

Bis(amino{[iminio(morpholino)methyl]amino}iminium) bis(amino{[imino(morpholino)methyl]amino}iminium) tetracosaoxidotellurohexamolybdate(6-) tetrahydrate

Crystal data

$(C_6H_{15}N_5O)_2(C_6H_{14}N_5O)_2[TeMo_6O_{24}].4H_2O$	F_{000} = 1820
M_r = 1850.21	D_x = 2.205 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 875 reflections
a = 15.722 (3) Å	θ = 3.1–25.0°
b = 9.2364 (18) Å	μ = 1.93 mm^{-1}
c = 19.256 (4) Å	T = 298 (2) K
β = 94.67 (3)°	Block, white
V = 2787.0 (10) Å^3	0.24 × 0.24 × 0.22 mm
Z = 2	

Data collection

Rigaku R-AXIS RAPID IP diffractometer	4883 independent reflections
Radiation source: fine-focus sealed tube	4465 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.030

Detector resolution: 0 pixels mm^{-1}

T = 298(2) K

ω scans

Absorption correction: multi-scan (ABSCOR; Higashi, 1995)

T_{min} = 0.643, T_{max} = 0.657

20771 measured reflections

θ_{max} = 25.0º

θ_{min} = 3.1º

h = −18→18

k = −10→10

l = −22→22

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.025

$wR(F^2)$ = 0.056

S = 1.09

4883 reflections

377 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0189P)^2 + 3.249P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.002

$\Delta\rho_{max}$ = 0.63 e Å^{-3}

$\Delta\rho_{min}$ = −0.86 e Å^{-3}

Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.00488 (13)

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Te1	1.0000	1.0000	0.0000	0.01336 (7)
Mo1	0.840705 (14)	0.97463 (2)	−0.121498 (12)	0.01725 (8)
Mo2	0.962462 (15)	1.03579 (3)	0.163987 (12)	0.01902 (8)
Mo3	0.804183 (14)	1.00883 (2)	0.045455 (12)	0.01829 (8)
O1	1.06718 (11)	0.87503 (19)	−0.05424 (9)	0.0177 (4)
O2	0.89805 (11)	0.88611 (19)	−0.01551 (9)	0.0166 (4)
O3	0.96442 (11)	1.09343 (19)	−0.08720 (9)	0.0176 (4)
O4	0.91282 (14)	1.1756 (2)	0.20215 (11)	0.0333 (5)
O5	0.92935 (12)	0.8616 (2)	−0.15719 (9)	0.0212 (4)

O6	0.75632 (13)	1.1543 (2)	0.08024 (11)	0.0330 (5)
O7	0.76252 (12)	0.8424 (2)	−0.12693 (11)	0.0276 (5)
O8	0.72660 (13)	0.8813 (2)	0.02944 (11)	0.0323 (5)
O9	0.99343 (13)	0.9194 (2)	0.22975 (10)	0.0296 (5)
O10	0.79802 (11)	1.09461 (19)	−0.04971 (9)	0.0192 (4)
O11	0.81680 (13)	1.0896 (2)	−0.18973 (10)	0.0293 (5)
O12	0.86502 (12)	0.9258 (2)	0.12556 (9)	0.0219 (4)
O13	0.51701 (15)	0.1569 (3)	−0.10142 (15)	0.0582 (8)
O14	0.70371 (14)	1.0881 (2)	0.31912 (13)	0.0397 (6)
O1W	0.96255 (14)	0.6375 (2)	0.11550 (12)	0.0370 (5)
H1	0.9889	0.7141	0.1055	0.044*
H2	0.9140	0.6556	0.1301	0.044*
O2W	1.07989 (17)	0.4426 (3)	0.18435 (15)	0.0540 (7)
H3	1.0676	0.3607	0.1661	0.065*
H4	1.0434	0.4979	0.1629	0.065*
N1	0.83492 (18)	0.6090 (3)	−0.03895 (14)	0.0344 (6)
H5	0.8712	0.6705	−0.0155	0.041*
H6	0.7979	0.6376	−0.0744	0.041*
N2	0.90623 (15)	0.4192 (3)	0.01555 (13)	0.0282 (6)
H7	0.9353	0.4823	0.0441	0.034*
H8	0.9136	0.3237	0.0232	0.034*
N3	0.79856 (16)	0.3705 (3)	−0.06762 (13)	0.0277 (6)
H9	0.8008	0.2776	−0.0534	0.033*
N4	0.75224 (18)	0.4803 (3)	−0.17227 (14)	0.0354 (6)
H10	0.8071	0.5025	−0.1774	0.042*
H11	0.7113	0.5017	−0.2061	0.042*
N5	0.65933 (16)	0.3408 (3)	−0.11197 (13)	0.0300 (6)
N6	1.0938 (2)	0.7734 (4)	0.45693 (18)	0.0577 (9)
H12	1.0669	0.7843	0.4961	0.069*
H13	1.1469	0.7363	0.4607	0.069*
N7	1.08581 (17)	0.7464 (3)	0.33860 (16)	0.0453 (8)
H14	1.1380	0.7059	0.3425	0.054*
H15	1.0642	0.7675	0.2950	0.054*
N8	0.96948 (16)	0.8341 (3)	0.39610 (14)	0.0358 (6)
N9	0.90343 (17)	0.6720 (3)	0.31506 (16)	0.0418 (7)
H16	0.9432	0.6051	0.3279	0.050*
H17	0.8657	0.6575	0.2780	0.050*
N10	0.84324 (15)	0.8936 (3)	0.33528 (13)	0.0263 (5)
C1	0.5878 (2)	0.1522 (4)	−0.05053 (19)	0.0438 (9)
H1A	0.6283	0.0799	−0.0637	0.053*
H1B	0.5684	0.1246	−0.0058	0.053*
C2	0.5475 (2)	0.1889 (5)	−0.1672 (2)	0.0537 (10)
H2A	0.4998	0.1879	−0.2026	0.064*
H2B	0.5872	0.1140	−0.1788	0.064*
C3	0.5913 (2)	0.3336 (4)	−0.16842 (18)	0.0416 (8)
H3A	0.6151	0.3470	−0.2129	0.050*
H3B	0.5502	0.4103	−0.1629	0.050*
C4	0.6308 (2)	0.2974 (4)	−0.04428 (17)	0.0381 (8)
H4A	0.5912	0.3689	−0.0288	0.046*

H4B	0.6794	0.2925	−0.0099	0.046*
C5	0.7344 (2)	0.4006 (3)	−0.11897 (15)	0.0263 (6)
C6	0.84770 (18)	0.4686 (3)	−0.03086 (15)	0.0228 (6)
C7	0.7724 (2)	1.1139 (4)	0.3706 (2)	0.0452 (9)
H7A	0.7575	1.0754	0.4149	0.054*
H7B	0.7806	1.2175	0.3761	0.054*
C8	0.6910 (2)	0.9357 (3)	0.31187 (19)	0.0371 (8)
H8A	0.6423	0.9178	0.2788	0.045*
H8B	0.6784	0.8954	0.3564	0.045*
C9	0.76780 (19)	0.8614 (4)	0.28752 (17)	0.0320 (7)
H9A	0.7582	0.7577	0.2858	0.038*
H9B	0.7774	0.8942	0.2409	0.038*
C10	0.8540 (2)	1.0472 (4)	0.35268 (18)	0.0367 (8)
H10A	0.8746	1.0980	0.3133	0.044*
H10B	0.8964	1.0573	0.3919	0.044*
C11	0.90742 (19)	0.8001 (3)	0.34730 (16)	0.0288 (7)
C12	1.0479 (2)	0.7821 (4)	0.39541 (19)	0.0372 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Te1	0.01484 (13)	0.01183 (12)	0.01295 (13)	−0.00084 (8)	−0.00163 (9)	0.00035 (9)
Mo1	0.01854 (13)	0.01554 (13)	0.01677 (13)	−0.00164 (9)	−0.00401 (9)	0.00015 (9)
Mo2	0.02178 (14)	0.02072 (14)	0.01437 (13)	−0.00030 (9)	0.00025 (9)	−0.00023 (9)
Mo3	0.01674 (13)	0.01865 (13)	0.01923 (13)	−0.00111 (9)	0.00005 (9)	0.00082 (9)
O1	0.0194 (9)	0.0156 (9)	0.0179 (9)	0.0014 (7)	0.0009 (7)	−0.0018 (8)
O2	0.0170 (9)	0.0144 (9)	0.0179 (9)	−0.0031 (7)	−0.0019 (7)	0.0007 (7)
O3	0.0196 (9)	0.0168 (9)	0.0157 (9)	−0.0010 (7)	−0.0036 (7)	0.0028 (8)
O4	0.0345 (12)	0.0342 (12)	0.0315 (11)	0.0043 (9)	0.0054 (9)	−0.0070 (10)
O5	0.0244 (10)	0.0188 (9)	0.0201 (9)	−0.0027 (8)	−0.0005 (8)	−0.0035 (8)
O6	0.0318 (12)	0.0371 (12)	0.0298 (11)	0.0105 (9)	0.0017 (9)	−0.0031 (10)
O7	0.0233 (10)	0.0250 (10)	0.0334 (11)	−0.0050 (8)	−0.0051 (9)	−0.0030 (9)
O8	0.0286 (12)	0.0341 (12)	0.0329 (11)	−0.0120 (9)	−0.0046 (9)	0.0071 (10)
O9	0.0335 (12)	0.0330 (12)	0.0216 (10)	−0.0047 (9)	−0.0028 (9)	0.0083 (9)
O10	0.0194 (10)	0.0149 (9)	0.0226 (9)	0.0018 (7)	−0.0021 (7)	0.0017 (8)
O11	0.0361 (12)	0.0257 (11)	0.0245 (11)	0.0008 (9)	−0.0077 (9)	0.0050 (9)
O12	0.0221 (10)	0.0234 (10)	0.0202 (10)	−0.0035 (8)	0.0014 (8)	0.0042 (8)
O13	0.0313 (14)	0.076 (2)	0.0657 (18)	−0.0082 (13)	−0.0048 (12)	0.0279 (16)
O14	0.0301 (12)	0.0254 (11)	0.0622 (16)	0.0041 (9)	−0.0047 (11)	0.0019 (11)
O1W	0.0405 (13)	0.0229 (11)	0.0482 (14)	−0.0051 (9)	0.0074 (11)	−0.0027 (11)
O2W	0.0557 (17)	0.0388 (14)	0.0658 (18)	−0.0077 (12)	−0.0047 (14)	0.0036 (14)
N1	0.0478 (17)	0.0171 (12)	0.0358 (15)	−0.0010 (11)	−0.0125 (12)	0.0008 (11)
N2	0.0320 (14)	0.0203 (12)	0.0307 (14)	−0.0021 (10)	−0.0074 (11)	0.0000 (11)
N3	0.0379 (15)	0.0123 (11)	0.0306 (13)	−0.0008 (10)	−0.0105 (11)	0.0038 (10)
N4	0.0389 (16)	0.0341 (15)	0.0312 (15)	−0.0047 (12)	−0.0085 (12)	0.0095 (12)
N5	0.0314 (14)	0.0328 (14)	0.0249 (13)	0.0016 (11)	−0.0042 (11)	0.0049 (11)
N6	0.0385 (18)	0.078 (2)	0.053 (2)	0.0157 (17)	−0.0173 (15)	0.0055 (19)
N7	0.0240 (15)	0.060 (2)	0.0519 (19)	0.0129 (13)	0.0017 (13)	0.0115 (16)

N8	0.0272 (14)	0.0463 (17)	0.0325 (14)	0.0086 (12)	−0.0049 (11)	−0.0024 (13)
N9	0.0308 (15)	0.0335 (15)	0.0598 (19)	0.0085 (12)	−0.0045 (14)	−0.0079 (14)
N10	0.0199 (12)	0.0285 (13)	0.0299 (13)	0.0014 (10)	−0.0011 (10)	−0.0025 (11)
C1	0.0363 (19)	0.052 (2)	0.043 (2)	0.0019 (16)	0.0027 (16)	0.0171 (18)
C2	0.041 (2)	0.068 (3)	0.049 (2)	−0.0111 (19)	−0.0164 (17)	0.012 (2)
C3	0.0325 (18)	0.055 (2)	0.0356 (18)	0.0014 (16)	−0.0110 (14)	0.0133 (17)
C4	0.0416 (19)	0.046 (2)	0.0274 (17)	0.0097 (15)	0.0064 (14)	0.0049 (16)
C5	0.0373 (17)	0.0163 (14)	0.0239 (15)	0.0037 (12)	−0.0062 (12)	0.0000 (12)
C6	0.0293 (15)	0.0156 (13)	0.0237 (14)	−0.0022 (11)	0.0028 (12)	0.0002 (12)
C7	0.044 (2)	0.0358 (19)	0.056 (2)	0.0023 (16)	0.0007 (17)	−0.0128 (18)
C8	0.0277 (17)	0.0307 (17)	0.052 (2)	0.0008 (13)	−0.0016 (15)	0.0033 (16)
C9	0.0257 (16)	0.0342 (17)	0.0352 (17)	−0.0002 (13)	−0.0037 (13)	−0.0047 (15)
C10	0.0341 (18)	0.0343 (18)	0.0407 (19)	−0.0018 (14)	−0.0024 (14)	−0.0083 (15)
C11	0.0226 (15)	0.0345 (17)	0.0295 (16)	0.0014 (12)	0.0040 (12)	0.0045 (14)
C12	0.0279 (17)	0.0330 (17)	0.049 (2)	0.0014 (14)	−0.0065 (15)	0.0101 (16)

Geometric parameters (Å, °)

Te1—O2	1.9202 (17)	N3—C5	1.382 (4)
Te1—O2^{i}	1.9202 (17)	N3—H9	0.9000
Te1—O1	1.9283 (17)	N4—C5	1.312 (4)
Te1—O1^{i}	1.9283 (17)	N4—H10	0.8998
Te1—O3	1.9298 (17)	N4—H11	0.9000
Te1—O3^{i}	1.9298 (17)	N5—C5	1.320 (4)
Mo1—O11	1.7075 (19)	N5—C3	1.464 (4)
Mo1—O7	1.7298 (19)	N5—C4	1.468 (4)
Mo1—O5	1.9131 (19)	N6—C12	1.339 (4)
Mo1—O10	1.9339 (18)	N6—H12	0.9001
Mo1—O3	2.2834 (18)	N6—H13	0.9000
Mo1—O2	2.3123 (18)	N7—C12	1.329 (4)
Mo2—O9	1.702 (2)	N7—H14	0.9001
Mo2—O4	1.706 (2)	N7—H15	0.9001
Mo2—O12	1.9343 (19)	N8—C12	1.324 (4)
Mo2—O5^{i}	1.9606 (19)	N8—C11	1.336 (4)
Mo2—O1^{i}	2.2806 (18)	N9—C11	1.335 (4)
Mo2—O3^{i}	2.2823 (18)	N9—H16	0.8999
Mo3—O6	1.704 (2)	N9—H17	0.9000
Mo3—O8	1.706 (2)	N10—C11	1.334 (4)
Mo3—O12	1.9084 (19)	N10—C10	1.464 (4)
Mo3—O10	1.9916 (18)	N10—C9	1.471 (4)
Mo3—O2	2.2634 (18)	C1—C4	1.503 (5)
Mo3—O1^{i}	2.2835 (18)	C1—H1A	0.9700
O1—Mo2^{i}	2.2806 (18)	C1—H1B	0.9700
O1—Mo3^{i}	2.2835 (18)	C2—C3	1.504 (5)
O3—Mo2^{i}	2.2823 (18)	C2—H2A	0.9700
O5—Mo2^{i}	1.9606 (18)	C2—H2B	0.9700
O13—C2	1.422 (5)	C3—H3A	0.9700

O13—C1	1.422 (4)	C3—H3B	0.9700
O14—C7	1.426 (4)	C4—H4A	0.9700
O14—C8	1.427 (4)	C4—H4B	0.9700
O1W—H1	0.8500	C7—C10	1.488 (5)
O1W—H2	0.8500	C7—H7A	0.9700
O2W—H3	0.8499	C7—H7B	0.9700
O2W—H4	0.8500	C8—C9	1.497 (4)
N1—C6	1.319 (4)	C8—H8A	0.9700
N1—H5	0.8999	C8—H8B	0.9700
N1—H6	0.9001	C9—H9A	0.9700
N2—C6	1.311 (4)	C9—H9B	0.9700
N2—H7	0.9001	C10—H10A	0.9700
N2—H8	0.9000	C10—H10B	0.9700
N3—C6	1.353 (4)		
O2—Te1—O2^{i}	180.0	C6—N3—C5	126.3 (2)
O2—Te1—O1	94.30 (8)	C6—N3—H9	118.2
O2^{i}—Te1—O1	85.70 (8)	C5—N3—H9	114.6
O2—Te1—O1^{i}	85.70 (8)	C5—N4—H10	118.8
O2^{i}—Te1—O1^{i}	94.30 (8)	C5—N4—H11	120.2
O1—Te1—O1^{i}	180.00 (8)	H10—N4—H11	120.5
O2—Te1—O3	86.01 (8)	C5—N5—C3	123.3 (3)
O2^{i}—Te1—O3	93.99 (8)	C5—N5—C4	123.1 (3)
O1—Te1—O3	85.94 (8)	C3—N5—C4	112.9 (3)
O1^{i}—Te1—O3	94.06 (8)	C12—N6—H12	118.6
O2—Te1—O3^{i}	93.99 (8)	C12—N6—H13	121.6
O2^{i}—Te1—O3^{i}	86.01 (8)	H12—N6—H13	118.1
O1—Te1—O3^{i}	94.06 (8)	C12—N7—H14	120.1
O1^{i}—Te1—O3^{i}	85.94 (8)	C12—N7—H15	123.6
O3—Te1—O3^{i}	180.00 (10)	H14—N7—H15	116.1
O11—Mo1—O7	106.37 (10)	C12—N8—C11	122.3 (3)
O11—Mo1—O5	100.61 (9)	C11—N9—H16	118.4
O7—Mo1—O5	97.36 (9)	C11—N9—H17	120.3
O11—Mo1—O10	97.24 (9)	H16—N9—H17	120.9
O7—Mo1—O10	99.29 (9)	C11—N10—C10	121.1 (3)
O5—Mo1—O10	151.01 (8)	C11—N10—C9	122.5 (3)
O11—Mo1—O3	93.01 (9)	C10—N10—C9	114.3 (2)
O7—Mo1—O3	160.24 (8)	O13—C1—C4	110.4 (3)
O5—Mo1—O3	74.79 (7)	O13—C1—H1A	109.6
O10—Mo1—O3	81.66 (7)	C4—C1—H1A	109.6
O11—Mo1—O2	160.86 (8)	O13—C1—H1B	109.6
O7—Mo1—O2	91.60 (8)	C4—C1—H1B	109.6
O5—Mo1—O2	83.17 (7)	H1A—C1—H1B	108.1
O10—Mo1—O2	72.83 (7)	O13—C2—C3	112.7 (3)
O3—Mo1—O2	69.69 (6)	O13—C2—H2A	109.1
O9—Mo2—O4	105.72 (10)	C3—C2—H2A	109.1
O9—Mo2—O12	97.04 (9)	O13—C2—H2B	109.1

O4—Mo2—O12	100.74 (9)	C3—C2—H2B	109.1
O9—Mo2—O5^{i}	99.08 (9)	H2A—C2—H2B	107.8
O4—Mo2—O5^{i}	95.33 (9)	N5—C3—C2	109.7 (3)
O12—Mo2—O5^{i}	153.20 (8)	N5—C3—H3A	109.7
O9—Mo2—O1^{i}	160.41 (8)	C2—C3—H3A	109.7
O4—Mo2—O1^{i}	93.42 (9)	N5—C3—H3B	109.7
O12—Mo2—O1^{i}	74.90 (7)	C2—C3—H3B	109.7
O5^{i}—Mo2—O1^{i}	82.91 (7)	H3A—C3—H3B	108.2
O9—Mo2—O3^{i}	91.31 (9)	N5—C4—C1	109.9 (3)
O4—Mo2—O3^{i}	161.30 (9)	N5—C4—H4A	109.7
O12—Mo2—O3^{i}	84.42 (7)	C1—C4—H4A	109.7
O5^{i}—Mo2—O3^{i}	73.98 (7)	N5—C4—H4B	109.7
O1^{i}—Mo2—O3^{i}	70.38 (6)	C1—C4—H4B	109.7
O6—Mo3—O8	106.47 (11)	H4A—C4—H4B	108.2
O6—Mo3—O12	101.97 (9)	N4—C5—N5	124.4 (3)
O8—Mo3—O12	99.94 (9)	N4—C5—N3	118.8 (3)
O6—Mo3—O10	93.33 (9)	N5—C5—N3	116.7 (3)
O8—Mo3—O10	97.35 (9)	N2—C6—N1	121.0 (3)
O12—Mo3—O10	152.52 (8)	N2—C6—N3	117.5 (3)
O6—Mo3—O2	157.88 (9)	N1—C6—N3	121.4 (3)
O8—Mo3—O2	92.71 (9)	O14—C7—C10	112.8 (3)
O12—Mo3—O2	85.01 (7)	O14—C7—H7A	109.0
O10—Mo3—O2	72.96 (7)	C10—C7—H7A	109.0
O6—Mo3—O1^{i}	90.99 (9)	O14—C7—H7B	109.0
O8—Mo3—O1^{i}	162.53 (9)	C10—C7—H7B	109.0
O12—Mo3—O1^{i}	75.30 (7)	H7A—C7—H7B	107.8
O10—Mo3—O1^{i}	81.82 (7)	O14—C8—C9	111.9 (3)
O2—Mo3—O1^{i}	70.29 (6)	O14—C8—H8A	109.2
Te1—O1—Mo2^{i}	101.89 (8)	C9—C8—H8A	109.2
Te1—O1—Mo3^{i}	101.51 (8)	O14—C8—H8B	109.2
Mo2^{i}—O1—Mo3^{i}	90.68 (7)	C9—C8—H8B	109.2
Te1—O2—Mo3	102.49 (8)	H8A—C8—H8B	107.9
Te1—O2—Mo1	101.78 (8)	N10—C9—C8	110.0 (3)
Mo3—O2—Mo1	93.26 (7)	N10—C9—H9A	109.7
Te1—O3—Mo2^{i}	101.78 (8)	C8—C9—H9A	109.7
Te1—O3—Mo1	102.51 (8)	N10—C9—H9B	109.7
Mo2^{i}—O3—Mo1	91.35 (6)	C8—C9—H9B	109.7
Mo1—O5—Mo2^{i}	114.94 (9)	H9A—C9—H9B	108.2
Mo1—O10—Mo3	115.85 (9)	N10—C10—C7	111.7 (3)
Mo3—O12—Mo2	115.31 (9)	N10—C10—H10A	109.3
C2—O13—C1	108.6 (3)	C7—C10—H10A	109.3
C7—O14—C8	109.0 (2)	N10—C10—H10B	109.3
H1—O1W—H2	112.3	C7—C10—H10B	109.3
H3—O2W—H4	102.2	H10A—C10—H10B	107.9

C6—N1—H5	118.5	N10—C11—N9	119.1 (3)
C6—N1—H6	117.5	N10—C11—N8	118.0 (3)
H5—N1—H6	122.6	N9—C11—N8	122.6 (3)
C6—N2—H7	119.0	N8—C12—N7	125.3 (3)
C6—N2—H8	121.8	N8—C12—N6	116.6 (3)
H7—N2—H8	118.8	N7—C12—N6	117.9 (3)
O2—Te1—O1—Mo2^{i}	86.08 (8)	O10—Mo1—O5—Mo2^{i}	−56.2 (2)
O2^{i}—Te1—O1—Mo2^{i}	−93.92 (8)	O3—Mo1—O5—Mo2^{i}	−19.37 (8)
O3—Te1—O1—Mo2^{i}	0.40 (7)	O2—Mo1—O5—Mo2^{i}	−90.12 (10)
O3^{i}—Te1—O1—Mo2^{i}	−179.60 (7)	O11—Mo1—O10—Mo3	177.24 (10)
O2—Te1—O1—Mo3^{i}	179.25 (7)	O7—Mo1—O10—Mo3	69.26 (11)
O2^{i}—Te1—O1—Mo3^{i}	−0.75 (7)	O5—Mo1—O10—Mo3	−55.0 (2)
O3—Te1—O1—Mo3^{i}	93.57 (8)	O3—Mo1—O10—Mo3	−90.76 (10)
O3^{i}—Te1—O1—Mo3^{i}	−86.43 (8)	O2—Mo1—O10—Mo3	−19.54 (8)
O1—Te1—O2—Mo3	179.24 (7)	O6—Mo3—O10—Mo1	−177.72 (11)
O1^{i}—Te1—O2—Mo3	−0.76 (7)	O8—Mo3—O10—Mo1	−70.63 (12)
O3—Te1—O2—Mo3	−95.14 (8)	O12—Mo3—O10—Mo1	58.1 (2)
O3^{i}—Te1—O2—Mo3	84.86 (8)	O2—Mo3—O10—Mo1	19.96 (8)
O1—Te1—O2—Mo1	−84.69 (8)	O1^{i}—Mo3—O10—Mo1	91.76 (10)
O1^{i}—Te1—O2—Mo1	95.31 (8)	O6—Mo3—O12—Mo2	−70.74 (12)
O3—Te1—O2—Mo1	0.92 (7)	O8—Mo3—O12—Mo2	179.91 (11)
O3^{i}—Te1—O2—Mo1	−179.08 (7)	O10—Mo3—O12—Mo2	51.7 (2)
O6—Mo3—O2—Te1	34.3 (3)	O2—Mo3—O12—Mo2	88.02 (10)
O8—Mo3—O2—Te1	−175.22 (9)	O1^{i}—Mo3—O12—Mo2	17.12 (9)
O12—Mo3—O2—Te1	−75.47 (8)	O9—Mo2—O12—Mo3	−178.97 (11)
O10—Mo3—O2—Te1	87.92 (9)	O4—Mo2—O12—Mo3	73.50 (12)
O1^{i}—Mo3—O2—Te1	0.68 (6)	O5^{i}—Mo2—O12—Mo3	−52.3 (2)
O6—Mo3—O2—Mo1	−68.6 (2)	O1^{i}—Mo2—O12—Mo3	−17.17 (9)
O8—Mo3—O2—Mo1	81.95 (9)	O3^{i}—Mo2—O12—Mo3	−88.33 (10)
O12—Mo3—O2—Mo1	−178.30 (7)	C2—O13—C1—C4	62.7 (4)
O10—Mo3—O2—Mo1	−14.91 (6)	C1—O13—C2—C3	−61.4 (4)
O1^{i}—Mo3—O2—Mo1	−102.15 (7)	C5—N5—C3—C2	140.0 (3)
O11—Mo1—O2—Te1	−27.3 (3)	C4—N5—C3—C2	−49.8 (4)
O7—Mo1—O2—Te1	172.66 (9)	O13—C2—C3—N5	54.6 (4)
O5—Mo1—O2—Te1	75.44 (8)	C5—N5—C4—C1	−137.4 (3)
O10—Mo1—O2—Te1	−88.10 (9)	C3—N5—C4—C1	52.3 (4)
O3—Mo1—O2—Te1	−0.83 (6)	O13—C1—C4—N5	−58.5 (4)
O11—Mo1—O2—Mo3	76.2 (3)	C3—N5—C5—N4	11.6 (5)
O7—Mo1—O2—Mo3	−83.85 (8)	C4—N5—C5—N4	−157.6 (3)
O5—Mo1—O2—Mo3	178.93 (7)	C3—N5—C5—N3	−165.4 (3)
O10—Mo1—O2—Mo3	15.38 (6)	C4—N5—C5—N3	25.3 (4)
O3—Mo1—O2—Mo3	102.65 (7)	C6—N3—C5—N4	55.3 (4)
O2—Te1—O3—Mo2^{i}	−95.00 (8)	C6—N3—C5—N5	−127.5 (3)
O2^{i}—Te1—O3—Mo2^{i}	85.00 (8)	C5—N3—C6—N2	−179.4 (3)

O1—Te1—O3—Mo2^{i}	−0.40 (7)	C5—N3—C6—N1	3.6 (5)
O1^{i}—Te1—O3—Mo2^{i}	179.60 (7)	C8—O14—C7—C10	59.6 (4)
O2—Te1—O3—Mo1	−0.94 (7)	C7—O14—C8—C9	−62.0 (4)
O2^{i}—Te1—O3—Mo1	179.06 (7)	C11—N10—C9—C8	148.7 (3)
O1—Te1—O3—Mo1	93.67 (8)	C10—N10—C9—C8	−47.8 (4)
O1^{i}—Te1—O3—Mo1	−86.33 (8)	O14—C8—C9—N10	56.0 (4)
O11—Mo1—O3—Te1	172.42 (9)	C11—N10—C10—C7	−150.2 (3)
O7—Mo1—O3—Te1	−18.7 (3)	C9—N10—C10—C7	46.0 (4)
O5—Mo1—O3—Te1	−87.41 (9)	O14—C7—C10—N10	−51.7 (4)
O10—Mo1—O3—Te1	75.53 (8)	C10—N10—C11—N9	−162.6 (3)
O2—Mo1—O3—Te1	0.83 (6)	C9—N10—C11—N9	−0.1 (4)
O11—Mo1—O3—Mo2^{i}	−85.20 (9)	C10—N10—C11—N8	23.3 (4)
O7—Mo1—O3—Mo2^{i}	83.6 (2)	C9—N10—C11—N8	−174.2 (3)
O5—Mo1—O3—Mo2^{i}	14.98 (7)	C12—N8—C11—N10	−154.6 (3)
O10—Mo1—O3—Mo2^{i}	177.91 (7)	C12—N8—C11—N9	31.6 (5)
O2—Mo1—O3—Mo2^{i}	103.21 (7)	C11—N8—C12—N7	30.2 (5)
O11—Mo1—O5—Mo2^{i}	70.89 (11)	C11—N8—C12—N6	−154.1 (3)
O7—Mo1—O5—Mo2^{i}	179.14 (10)		

Symmetry codes: (i) −*x*+2, −*y*+2, −*z*.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H6···O7	0.90	2.20	2.916 (3)	137
N1—H5···O2	0.90	2.04	2.769 (3)	138
N2—H8···O1^{ii}	0.90	1.95	2.840 (3)	172
N2—H7···O1W	0.90	2.01	2.877 (3)	162
N3—H9···O10^{iii}	0.90	1.69	2.571 (3)	165
N4—H11···O11^{iv}	0.90	2.18	2.965 (3)	146
N4—H10···O2W^{ii}	0.90	1.86	2.762 (4)	177
N9—H17···O14^{v}	0.90	2.18	3.067 (4)	167
N7—H15···O9	0.90	2.14	2.925 (4)	146
N7—H14···O7^{vi}	0.90	2.05	2.921 (3)	164
N6—H13···O8^{vi}	0.90	2.06	2.806 (4)	140
O1W—H1···O3^{i}	0.85	1.97	2.810 (3)	172
O1W—H2···O12	0.85	2.61	3.087 (3)	117
O1W—H2···O14^{v}	0.85	2.25	3.027 (3)	152
O2W—H3···O5^{ii}	0.85	2.06	2.860 (3)	156
O2W—H4···O1W	0.85	1.98	2.829 (4)	176

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

Fig. 1

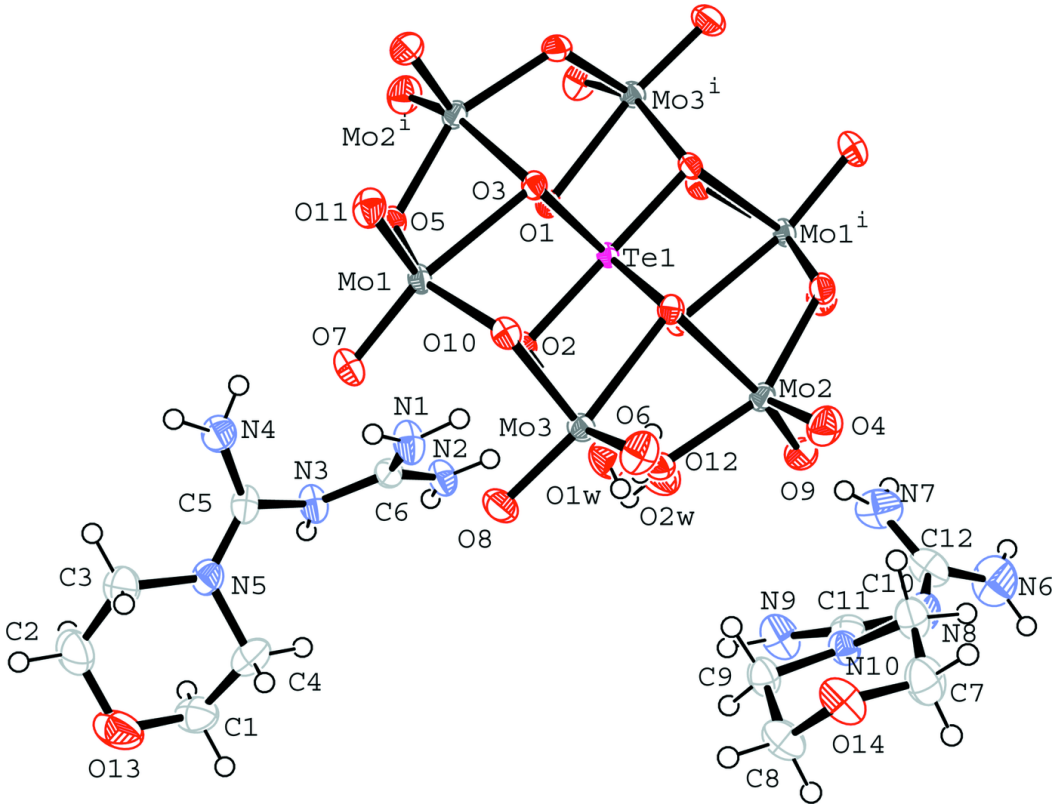
Mo3i
Mo2i
O3
O11
O5
O1
Mo1i
Te1
Mo1
O7
O10
O2
Mo2
N1
N4
Mo3
O6
O4
N2
N3
O12
C5
C6
O1w
O2w
O9
N7
O8
C12
C3
N5
C10
N6
N9
C11
C2
N8
N10
C9
C4
C7
C1
O14
O13
C8

Fig. 2

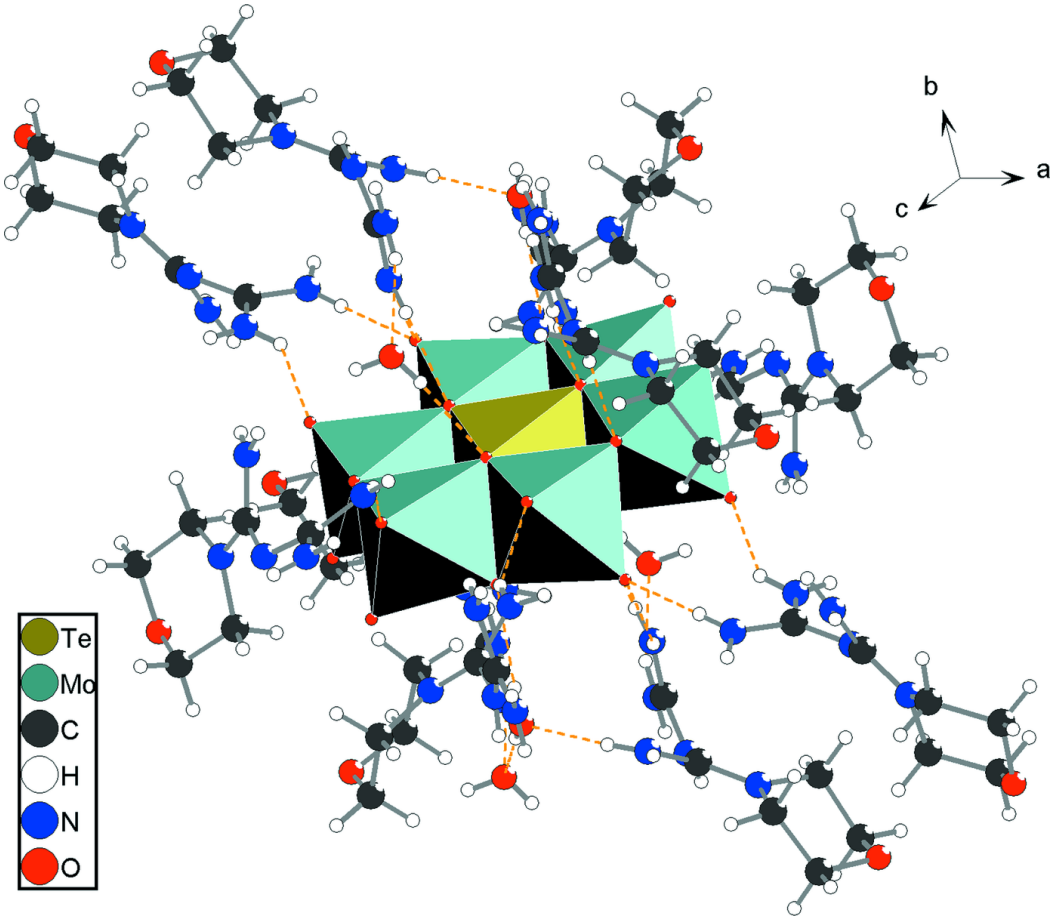

Fig. 3