

Tetraquatetrakis(4,4'-bipyridine dioxido- κ O)terbium(III) octacyanidomolybdate(V)

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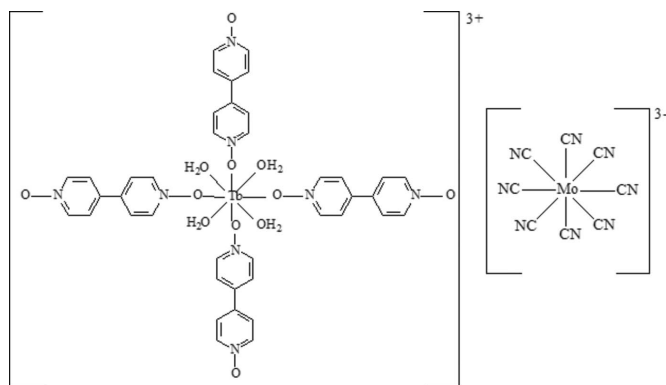
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Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.016; wR factor = 0.043; data-to-parameter ratio = 16.5.

In the title compound, $[\text{Tb}(\text{C}_{10}\text{H}_8\text{N}_2\text{O}_2)_4(\text{H}_2\text{O})_4][\text{Mo}(\text{CN})_8]$, both metal atoms are eight-coordinated. The Tb^{III} atom displays a dodecahedral geometry, while the Mo^{V} ion exhibits a distorted square-antiprismatic geometry. The Tb atoms are located on a special position of site symmetry $\bar{4}$, whereas the Mo atoms are located on a twofold rotation axis. The cations are linked by $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds.

Related literature

For general background to octacyanidometallate-based complexes involving lanthanide ions, see: Chelebaeva *et al.* (2009); Ma *et al.* (2009); Qian *et al.* (2010); Wang *et al.* (2006); Zhou *et al.* (2010). For the preparation of the title compound, see: Bok *et al.* (1975). For related structures, see: Koziel *et al.* (2010); Przychodzeń *et al.* (2007).



Experimental

Crystal data

$[\text{Tb}(\text{C}_{10}\text{H}_8\text{N}_2\text{O}_2)_4(\text{H}_2\text{O})_4]\text{Mo}(\text{CN})_8$	$V = 2533.7(2) \text{ \AA}^3$
$M_r = 1287.72$	$Z = 2$
Tetragonal, $P4/n$	Mo $K\alpha$ radiation
$a = 17.9226(7) \text{ \AA}$	$\mu = 1.71 \text{ mm}^{-1}$
$c = 7.8877(6) \text{ \AA}$	$T = 291 \text{ K}$
	$0.22 \times 0.21 \times 0.12 \text{ mm}$

Data collection

Bruker SMART APEX CCD diffractometer	21243 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2004)	2921 independent reflections
$T_{\text{min}} = 0.693$, $T_{\text{max}} = 0.843$	2730 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.016$	177 parameters
$wR(F^2) = 0.043$	H-atom parameters constrained
$S = 1.08$	$\Delta\rho_{\text{max}} = 0.36 \text{ e \AA}^{-3}$
2921 reflections	$\Delta\rho_{\text{min}} = -0.29 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O3}-\text{H3WA}\cdots\text{O2}^{\text{i}}$	0.83	1.85	2.6702 (15)	169
$\text{O3}-\text{H3WB}\cdots\text{O2}^{\text{ii}}$	0.84	1.92	2.7417 (16)	164

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

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: DIAMOND (Brandenburg, 2006); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5505).

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supplementary materials

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Tetraaquatetrakis(4,4'-bipyridine dioxide- κO)terbium(III) octacyanidomolybdate(V)

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Comment

In the past few years, octacyanomolybdate-based complexes have attracted considerable attention in the field of cyanide-bridged hetero-metallic system. Many assemblies based on $[M^V(CN)_8]^{3-}$ ($M = Mo$ or W) and lanthanide ions can take a variety of structures (Chelebaeva *et al.*, 2009; Koziel *et al.*, 2010; Ma *et al.*, 2009; Przychodzeń *et al.*, 2007; Qian *et al.*, 2010; Wang *et al.*, 2006; Zhou *et al.*, 2010). Recently, we have used $[Mo(CN)_8]^{3-}$ as a building block to react with Tb^{3+} and 4,4'-bipyridine dioxide (4,4'-dpdo) obtaining a new ionic complex, $[Tb(4,4'-bpdo)_4(H_2O)_4][Mo(CN)_8]$.

In the structure, the eight-coordinated Tb^{III} center displays a decahedron geometry, while each $[Mo^V(CN)_8]$ moiety exhibits a distorted square antiprismatic geometry. The average values of Mo—C and C—N bond distances are 2.171 and 1.155 Å, respectively, while the Mo—C—N units are nearly linear. The anions are linked by O—H...O hydrogen bonds.

Experimental

Single crystals of the title compound were prepared at room temperature in the dark by slow diffusion of a H_2O solution (3 ml) containing $Tb(NO_3)_3 \cdot 6H_2O$ (0.05 mmol) and 4,4'-dpdo (0.05 mmol) into a CH_3CN solution (15 ml) of $[HN(n-C_4H_9)_3]_3[Mo(CN)_8] \cdot 4H_2O$ (0.05 mmol) (Bok *et al.*, 1975). After two weeks, yellow block crystals were obtained.

Refinement

The H atoms of 4,4'-bipyridine dioxide ligands were ideally positioned with C—H = 0.93 Å and included in the refinement using a riding model with $U(H)$ set to 1.2 $U_{eq}(C)$. The H atoms bound to oxygen atoms were located from difference maps and refined as riding with $U(H)$ set to 1.2 $U_{eq}(O)$.

Figures

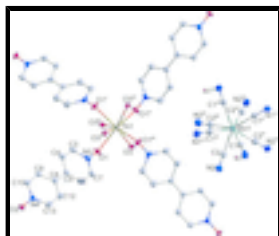


Fig. 1. ORTEP diagram of the title compound. Hydrogen atoms have been omitted for clarity and thermal ellipsoids are presented at the 30% probability level.

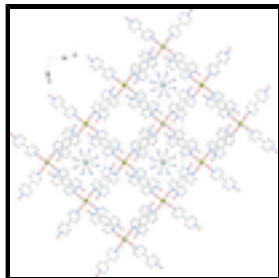


Fig. 2. Perspective view of the title compound in *ab* plane. Hydrogen atoms and coordinated water molecules have been omitted for clarity.

Tetraquatetrakis(4,4'-bipyridine dioxide- κ O)terbium(III) octacyanidomolybdate(V)

Crystal data

[Tb(C₁₀H₈N₂O₂)₄(H₂O)₄][Mo(CN)₈]

$M_r = 1287.72$

Tetragonal, *P4/n*

Hall symbol: -P 4a

$a = 17.9226$ (7) Å

$c = 7.8877$ (6) Å

$V = 2533.7$ (2) Å³

$Z = 2$

$F(000) = 1286$

$D_x = 1.688$ Mg m⁻³

Mo *K* α radiation, $\lambda = 0.71073$ Å

Cell parameters from 9881 reflections

$\theta = 2.3$ – 27.5°

$\mu = 1.71$ mm⁻¹

$T = 291$ K

Block, yellow

$0.22 \times 0.21 \times 0.12$ mm

Data collection

Bruker SMART APEX CCD
diffractometer

graphite

ϕ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2004)

$T_{\min} = 0.693$, $T_{\max} = 0.843$

21243 measured reflections

2921 independent reflections

2730 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 1.6^\circ$

$h = -23 \rightarrow 23$

$k = -23 \rightarrow 23$

$l = -10 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.016$

$wR(F^2) = 0.043$

$S = 1.08$

2921 reflections

177 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

$w = 1/[\sigma^2(F_o^2) + (0.0183P)^2 + 1.8165P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.36$ e Å⁻³

0 restraints

$$\Delta\rho_{\min} = -0.29 \text{ e } \text{\AA}^{-3}$$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Tb1	0.7500	0.2500	0.0000	0.01136 (5)
Mo1	0.7500	0.7500	-0.24987 (4)	0.02019 (7)
O1	0.64962 (6)	0.17736 (7)	0.10113 (14)	0.0251 (3)
O2	0.27973 (7)	-0.11246 (7)	-0.50459 (14)	0.0223 (2)
O3	0.70614 (6)	0.31664 (6)	0.24591 (13)	0.0183 (2)
N1	0.60473 (10)	0.81932 (10)	-0.4592 (3)	0.0422 (4)
N2	0.59644 (10)	0.70470 (10)	-0.0373 (3)	0.0393 (4)
N3	0.60104 (8)	0.13848 (8)	0.00837 (16)	0.0201 (3)
N4	0.33441 (7)	-0.07064 (7)	-0.44088 (17)	0.0176 (2)
C1	0.65693 (10)	0.79577 (9)	-0.3922 (3)	0.0300 (4)
C2	0.65123 (10)	0.71973 (9)	-0.1057 (3)	0.0293 (4)
C3	0.62224 (9)	0.07458 (9)	-0.0674 (2)	0.0234 (3)
H3	0.6709	0.0575	-0.0537	0.028*
C4	0.57297 (9)	0.03404 (9)	-0.1648 (2)	0.0215 (3)
H4	0.5888	-0.0098	-0.2166	0.026*
C5	0.49930 (8)	0.05822 (8)	-0.1867 (2)	0.0175 (3)
C6	0.47918 (9)	0.12409 (9)	-0.1031 (2)	0.0248 (3)
H6	0.4306	0.1419	-0.1129	0.030*
C7	0.53013 (10)	0.16301 (10)	-0.0063 (2)	0.0257 (4)
H7	0.5155	0.2064	0.0491	0.031*
C8	0.44383 (8)	0.01450 (8)	-0.28394 (19)	0.0168 (3)
C9	0.45913 (8)	-0.05724 (8)	-0.3460 (2)	0.0182 (3)
H9	0.5070	-0.0768	-0.3356	0.022*
C10	0.40389 (8)	-0.09908 (8)	-0.4224 (2)	0.0189 (3)
H10	0.4144	-0.1469	-0.4613	0.023*
C12	0.37208 (9)	0.04249 (8)	-0.3126 (2)	0.0209 (3)
H12	0.3604	0.0907	-0.2780	0.025*
C13	0.31847 (9)	-0.00028 (9)	-0.3913 (2)	0.0217 (3)
H13	0.2712	0.0193	-0.4103	0.026*
H3WA	0.6727	0.3040	0.3134	0.033*
H3WB	0.7363	0.3368	0.3136	0.033*

supplementary materials

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Tb1	0.01183 (5)	0.01183 (5)	0.01043 (7)	0.000	0.000	0.000
Mo1	0.01407 (8)	0.01407 (8)	0.03243 (15)	0.000	0.000	0.000
O1	0.0234 (6)	0.0348 (6)	0.0171 (5)	-0.0157 (5)	-0.0019 (5)	-0.0008 (5)
O2	0.0190 (5)	0.0247 (6)	0.0231 (6)	-0.0067 (4)	-0.0023 (4)	-0.0059 (4)
O3	0.0179 (5)	0.0232 (5)	0.0139 (5)	-0.0007 (4)	0.0019 (4)	-0.0032 (4)
N1	0.0310 (9)	0.0290 (8)	0.0666 (12)	-0.0020 (7)	-0.0123 (9)	0.0126 (8)
N2	0.0297 (8)	0.0313 (8)	0.0569 (11)	0.0000 (7)	0.0099 (8)	0.0101 (8)
N3	0.0188 (6)	0.0246 (7)	0.0170 (6)	-0.0095 (5)	-0.0005 (5)	0.0018 (5)
N4	0.0183 (6)	0.0198 (6)	0.0146 (6)	-0.0043 (5)	-0.0004 (5)	-0.0006 (5)
C1	0.0243 (8)	0.0195 (8)	0.0462 (11)	-0.0031 (6)	-0.0026 (8)	0.0050 (7)
C2	0.0241 (8)	0.0201 (8)	0.0438 (11)	0.0008 (6)	0.0020 (8)	0.0045 (7)
C3	0.0166 (7)	0.0280 (8)	0.0257 (8)	-0.0021 (6)	-0.0004 (6)	0.0010 (7)
C4	0.0189 (7)	0.0217 (7)	0.0239 (8)	-0.0016 (6)	0.0000 (6)	-0.0011 (6)
C5	0.0177 (7)	0.0172 (7)	0.0176 (7)	-0.0041 (5)	0.0004 (6)	0.0026 (6)
C6	0.0186 (7)	0.0210 (8)	0.0349 (9)	-0.0013 (6)	-0.0035 (7)	-0.0042 (7)
C7	0.0230 (8)	0.0215 (8)	0.0328 (9)	-0.0044 (6)	0.0002 (7)	-0.0052 (7)
C8	0.0173 (7)	0.0163 (7)	0.0168 (7)	-0.0037 (5)	0.0011 (5)	0.0019 (5)
C9	0.0162 (7)	0.0188 (7)	0.0198 (7)	-0.0004 (5)	0.0022 (6)	0.0009 (6)
C10	0.0203 (7)	0.0171 (7)	0.0191 (7)	-0.0006 (5)	0.0030 (6)	-0.0018 (6)
C12	0.0222 (7)	0.0166 (7)	0.0241 (8)	0.0009 (6)	-0.0023 (6)	-0.0016 (6)
C13	0.0192 (7)	0.0213 (7)	0.0246 (8)	0.0022 (6)	-0.0034 (6)	-0.0026 (6)

Geometric parameters (\AA , $^\circ$)

Tb1—O1 ⁱ	2.3596 (11)	N3—C3	1.346 (2)
Tb1—O1 ⁱⁱ	2.3596 (11)	N3—C7	1.350 (2)
Tb1—O1	2.3596 (11)	N4—C13	1.351 (2)
Tb1—O1 ⁱⁱⁱ	2.3596 (11)	N4—C10	1.3533 (19)
Tb1—O3 ⁱ	2.4097 (10)	C3—C4	1.378 (2)
Tb1—O3 ⁱⁱ	2.4097 (10)	C3—H3	0.9300
Tb1—O3	2.4097 (10)	C4—C5	1.400 (2)
Tb1—O3 ⁱⁱⁱ	2.4097 (10)	C4—H4	0.9300
Mo1—C1 ^{iv}	2.1715 (18)	C5—C6	1.400 (2)
Mo1—C1	2.1715 (18)	C5—C8	1.480 (2)
Mo1—C1 ^v	2.1715 (18)	C6—C7	1.379 (2)
Mo1—C1 ^{vi}	2.1715 (18)	C6—H6	0.9300
Mo1—C2 ^{iv}	2.1731 (18)	C7—H7	0.9300
Mo1—C2	2.1731 (18)	C8—C12	1.399 (2)
Mo1—C2 ^{vi}	2.1731 (18)	C8—C9	1.403 (2)
Mo1—C2 ^v	2.1731 (18)	C9—C10	1.380 (2)
O1—N3	1.3338 (17)	C9—H9	0.9300
O2—N4	1.3323 (16)	C10—H10	0.9300

O3—H3WA	0.8326	C12—C13	1.377 (2)
O3—H3WB	0.8422	C12—H12	0.9300
N1—C1	1.155 (2)	C13—H13	0.9300
N2—C2	1.152 (2)		
O1 ⁱ —Tb1—O1 ⁱⁱ	96.562 (17)	C1 ^{iv} —Mo1—C2 ^v	143.33 (6)
O1 ⁱ —Tb1—O1	96.562 (17)	C1—Mo1—C2 ^v	76.77 (7)
O1 ⁱⁱ —Tb1—O1	140.48 (5)	C1 ^v —Mo1—C2 ^v	74.88 (7)
O1 ⁱ —Tb1—O1 ⁱⁱⁱ	140.48 (5)	C1 ^{vi} —Mo1—C2 ^v	140.36 (6)
O1 ⁱⁱ —Tb1—O1 ⁱⁱⁱ	96.562 (17)	C2 ^{iv} —Mo1—C2 ^v	116.87 (11)
O1—Tb1—O1 ⁱⁱⁱ	96.562 (17)	C2—Mo1—C2 ^v	74.10 (5)
O1 ⁱ —Tb1—O3 ⁱ	75.68 (4)	C2 ^{vi} —Mo1—C2 ^v	74.10 (5)
O1 ⁱⁱ —Tb1—O3 ⁱ	146.10 (4)	N3—O1—Tb1	126.90 (9)
O1—Tb1—O3 ⁱ	73.39 (4)	Tb1—O3—H3WA	128.0
O1 ⁱⁱⁱ —Tb1—O3 ⁱ	72.73 (4)	Tb1—O3—H3WB	120.9
O1 ⁱ —Tb1—O3 ⁱⁱ	73.39 (4)	H3WA—O3—H3WB	100.0
O1 ⁱⁱ —Tb1—O3 ⁱⁱ	75.68 (4)	O1—N3—C3	120.24 (14)
O1—Tb1—O3 ⁱⁱ	72.73 (4)	O1—N3—C7	119.45 (14)
O1 ⁱⁱⁱ —Tb1—O3 ⁱⁱ	146.10 (4)	C3—N3—C7	120.30 (14)
O3 ⁱ —Tb1—O3 ⁱⁱ	130.38 (3)	O2—N4—C13	118.60 (13)
O1 ⁱ —Tb1—O3	146.10 (4)	O2—N4—C10	120.38 (13)
O1 ⁱⁱ —Tb1—O3	72.73 (4)	C13—N4—C10	121.00 (13)
O1—Tb1—O3	75.68 (4)	N1—C1—Mo1	175.79 (19)
O1 ⁱⁱⁱ —Tb1—O3	73.39 (4)	N2—C2—Mo1	176.07 (18)
O3 ⁱ —Tb1—O3	130.38 (3)	N3—C3—C4	121.02 (15)
O3 ⁱⁱ —Tb1—O3	72.79 (5)	N3—C3—H3	119.5
O1 ⁱ —Tb1—O3 ⁱⁱⁱ	72.73 (4)	C4—C3—H3	119.5
O1 ⁱⁱ —Tb1—O3 ⁱⁱⁱ	73.39 (4)	C3—C4—C5	120.65 (15)
O1—Tb1—O3 ⁱⁱⁱ	146.10 (4)	C3—C4—H4	119.7
O1 ⁱⁱⁱ —Tb1—O3 ⁱⁱⁱ	75.68 (4)	C5—C4—H4	119.7
O3 ⁱ —Tb1—O3 ⁱⁱⁱ	72.79 (5)	C6—C5—C4	116.49 (14)
O3 ⁱⁱ —Tb1—O3 ⁱⁱⁱ	130.38 (3)	C6—C5—C8	121.17 (14)
O3—Tb1—O3 ⁱⁱⁱ	130.38 (3)	C4—C5—C8	122.23 (14)
C1 ^{iv} —Mo1—C1	74.50 (5)	C7—C6—C5	121.10 (15)
C1 ^{iv} —Mo1—C1 ^v	117.74 (11)	C7—C6—H6	119.4
C1—Mo1—C1 ^v	74.50 (5)	C5—C6—H6	119.4
C1 ^{iv} —Mo1—C1 ^{vi}	74.50 (5)	N3—C7—C6	120.42 (16)
C1—Mo1—C1 ^{vi}	117.74 (11)	N3—C7—H7	119.8
C1 ^v —Mo1—C1 ^{vi}	74.50 (5)	C6—C7—H7	119.8
C1 ^{iv} —Mo1—C2 ^{iv}	74.88 (7)	C12—C8—C9	116.87 (14)
C1—Mo1—C2 ^{iv}	140.36 (6)	C12—C8—C5	120.77 (13)
C1 ^v —Mo1—C2 ^{iv}	143.33 (6)	C9—C8—C5	122.32 (13)

supplementary materials

C1 ^{vi} —Mo1—C2 ^{iv}	76.77 (7)	C10—C9—C8	120.66 (14)
C1 ^{iv} —Mo1—C2	76.77 (7)	C10—C9—H9	119.7
C1—Mo1—C2	74.88 (7)	C8—C9—H9	119.7
C1 ^v —Mo1—C2	140.36 (6)	N4—C10—C9	120.16 (14)
C1 ^{vi} —Mo1—C2	143.33 (6)	N4—C10—H10	119.9
C2 ^{iv} —Mo1—C2	74.10 (5)	C9—C10—H10	119.9
C1 ^{iv} —Mo1—C2 ^{vi}	140.36 (6)	C13—C12—C8	120.98 (14)
C1—Mo1—C2 ^{vi}	143.33 (6)	C13—C12—H12	119.5
C1 ^v —Mo1—C2 ^{vi}	76.77 (7)	C8—C12—H12	119.5
C1 ^{vi} —Mo1—C2 ^{vi}	74.88 (7)	N4—C13—C12	120.17 (14)
C2 ^{iv} —Mo1—C2 ^{vi}	74.10 (5)	N4—C13—H13	119.9
C2—Mo1—C2 ^{vi}	116.87 (11)	C12—C13—H13	119.9

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O3—H3WA \cdots O2 ^{vii}	0.83	1.85	2.6702 (15)	169
O3—H3WB \cdots O2 ^{viii}	0.84	1.92	2.7417 (16)	164
O3—H3WB \cdots N4 ^{viii}	0.84	2.62	3.4251 (16)	161

Symmetry codes: (vii) $-y+1/2, x, z+1$; (viii) $x+1/2, y+1/2, -z$.

Fig. 1

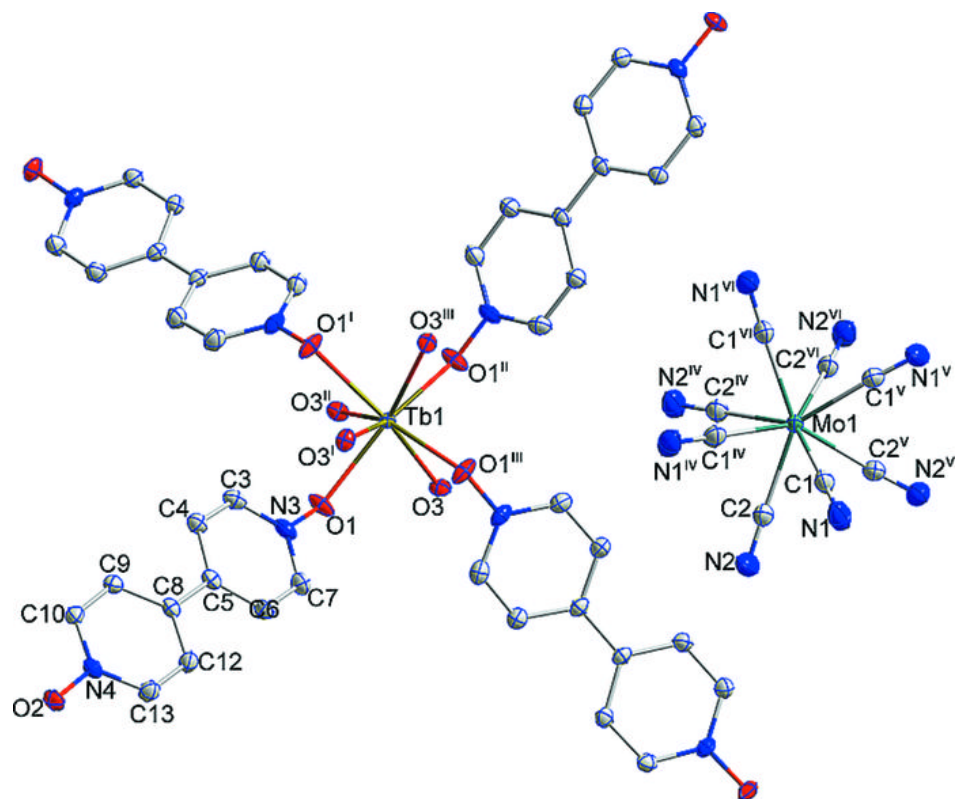


Fig. 2

