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Octakis[2,2',5,5'-tetrathiafulvalenium(0.5+)] bis[hexamolybdate(2-)] acetonitrile solvate

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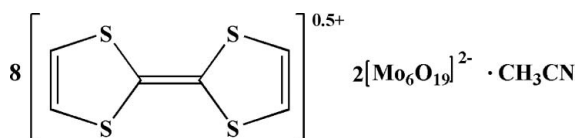
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.036; wR factor = 0.073; data-to-parameter ratio = 17.8.

The asymmetric unit of the title compound, $(\text{C}_6\text{H}_4\text{S}_4)_8\text{[Mo}_6\text{O}_{19}]_2 \cdot 2\text{CH}_3\text{CN}$, contains two halves of two centrosymmetric $[\text{Mo}_6\text{O}_{19}]^{2-}$ hexamolybdate anions, which are each built up from six distorted MoO_6 octahedra sharing common edges and one common vertex at the central O atom, six tetrathiafulvalene cations (three of which are located on mirror planes) to balance the charge and a half of an acetonitrile solvent molecule, likewise located on a mirror plane. The two central hexamolybdate O atoms occupy special positions 2*a* and 2*d*, respectively. The cations and anions are interlinked through $\text{C}-\text{H} \cdots \text{O}$ contacts.

Related literature

For the chemical and physical properties of polyoxomolybdates, see: Shi *et al.* (2006); Wang *et al.* (2004); Hagrman *et al.* (1999). For the structure of ammonium tris(tetraethylammonium) hexacosaoxidooctamolybdate, see: Zebiri *et al.* (2008). The title compound is isostructural with its tungsten analogue, see: Triki *et al.* (1993). The structure of the anions is the same as that in bis[2-(pyrimidin-2-ylamino)pyrimidinium] hexamolybdate, see: Yeh *et al.* (2008). For Mo—O distances, see: Boyle *et al.* (1998); Deng *et al.* (2006); Maeda *et al.* (2006).



Experimental

Crystal data

$(\text{C}_6\text{H}_4\text{S}_4)_8[\text{Mo}_6\text{O}_{19}]_2 \cdot 2\text{C}_2\text{H}_3\text{N}$
 $M_r = 3434.99$
 Monoclinic, $P2_1/m$

$a = 14.3179$ (8) Å
 $b = 20.2299$ (10) Å
 $c = 16.7625$ (10) Å

$\beta = 101.266$ (3)°
 $V = 4761.7$ (5) Å³
 $Z = 2$
 Mo $K\alpha$ radiation

$\mu = 2.31$ mm⁻¹
 $T = 100$ K
 $0.25 \times 0.15 \times 0.10$ mm

Data collection

Nonius KappaCCD diffractometer
 Absorption correction: multi-scan
 (*SADABS*; Sheldrick, 1996)
 $T_{\min} = 0.597$, $T_{\max} = 0.802$

45527 measured reflections
 11170 independent reflections
 8144 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.072$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.073$
 $S = 1$
 11170 reflections

629 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.88$ e Å⁻³
 $\Delta\rho_{\min} = -0.70$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H} \cdots A$	$D-\text{H}$	$\text{H} \cdots A$	$D \cdots A$	$D-\text{H} \cdots A$
$\text{C5}-\text{H5} \cdots \text{O11}^{\text{i}}$	0.93	2.28	3.192 (6)	167
$\text{C7}-\text{H7} \cdots \text{O19}^{\text{ii}}$	0.93	2.47	3.251 (7)	141
$\text{C7}-\text{H7} \cdots \text{O19}^{\text{iii}}$	0.93	2.47	3.251 (7)	141
$\text{C9}-\text{H9} \cdots \text{O12}$	0.93	2.54	3.388 (5)	151
$\text{C13}-\text{H13} \cdots \text{O17}^{\text{iv}}$	0.93	2.41	3.239 (6)	149
$\text{C14}-\text{H14} \cdots \text{O19}^{\text{v}}$	0.93	2.59	3.175 (5)	121
$\text{C18}-\text{H18} \cdots \text{O18}^{\text{vi}}$	0.93	2.41	3.145 (5)	136
$\text{C19}-\text{H19} \cdots \text{O10}^{\text{vii}}$	0.93	2.41	3.298 (5)	160
$\text{C20}-\text{H20} \cdots \text{O12}$	0.93	2.54	3.437 (5)	162
$\text{C24}-\text{H24} \cdots \text{O8}^{\text{viii}}$	0.93	2.25	3.075 (6)	148
$\text{C28}-\text{H28} \cdots \text{O4}^{\text{viii}}$	0.93	2.53	3.384 (6)	152
$\text{C29}-\text{H29} \cdots \text{O5}^{\text{viii}}$	0.93	2.52	3.256 (6)	137
$\text{C29}-\text{H29} \cdots \text{O6}^{\text{viii}}$	0.93	2.55	3.284 (6)	136

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

Data collection: *COLLECT* (Nonius, 2002); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PARST* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HG2545).

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supplementary materials

Acta Cryst. (2009). E65, m1063-m1064 [doi:10.1107/S1600536809031092]

Octakis[2,2',5,5'-tetrathiafulvalenium(0.5+)] bis[hexamolybdate(2-)] acetonitrile solvate

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Comment

As part of an ongoing study of materials containing polyoxomolybdates, we have just recently determined the structure of ammonium tris(tetraethylammonium) hexacosaoxidooctamolybdate (Zebiri *et al.*, 2008). These materials show interesting chemical and physical properties (Shi *et al.*, 2006; Wang, *et al.*, 2004; Hagrman, *et al.*, 1999).

The asymmetric unit of the title compound consists of a half neutral acetonitrile; two hexamolybdate anions and six tetrathiafulvalene in which two ones are (+1) charged and the rest ones with +0.5 charge (Fig. 1). The title compound is isostructural to (TTF)₄W₆O₁₉.0.5(CH₃CN) reported by Triki *et al.* (1993). The structure of the anions, as reported recently in Bis[2-(pyrimidin-2-ylamino)pyrimidinium] hexamolybdate (Yeh *et al.*, 2008), is constructed from an array of six edge-shared MoO₆ octahedra with six O(*t*), ten O(μ 2) and one O(μ 6) atoms.

The Mo—O distances, ranging from 1.681 (3) to 2.3363 (4) Å, agree with those reported for other [Mo₆O₁₉]²⁻ anions in the literature (Deng *et al.*, 2006; Maeda *et al.*, 2006; Boyle *et al.*, 1998) and can be grouped into three sets bridging groups [Mo—O(terminal) 1.681 (3)–1.696 (3) Å, Mo—O(μ 2): 1.850 (3)–2.027 (3) (1) Å and Mo—O(μ 6): 2.3151 (4) (1)–2.3363 (4) (1) Å.

Hexamolybdate anions spread along the *b* axis (Fig. 2) between which organic moieties intercalate. The cations and anions are interlinked through C—H \cdots O contacts.

Experimental

Single crystals of the title compound were prepared from a mixture of (NH₄)₆Mo₇O₂₄. 1.5 H₂O (137 mg, 1 mmol), C₆S₄H₄ (TTF) (612 mg, 3 mmol) and 3 ml H₂O, heated in a Teflon-lined steel autoclave inside a programmable electric furnace at 160 °C for 3 days. After cooling the autoclave to room temperature for 72 h, colorless crystals were obtained, filtered, washed with H₂O, EtOH, Et₂O and dried in air.

Refinement

H atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The methyl H atoms were constrained to an ideal geometry (C—H = 0.96 Å) with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$, but were allowed to rotate freely about the C—C bonds.

Figures

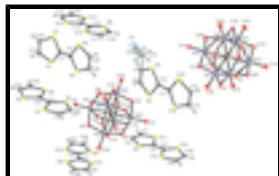


Fig. 1. The independent components of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level.

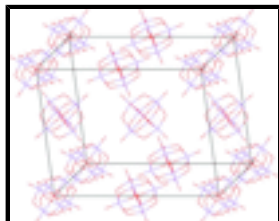


Fig. 2. hexamolybdate anions positions on the unit cell.

Octakis[2,2',5,5'-tetrathiafulvalenium(0.5+)] bis[hexamolybdate(2-)] acetonitrile solvate

Crystal data

$(C_6H_4S_4)_8[Mo_6O_{19}]_2 \cdot C_2H_3N$

$M_r = 3434.99$

Monoclinic, $P2_1/m$

Hall symbol: -P 2yb

$a = 14.3179$ (8) Å

$b = 20.2299$ (10) Å

$c = 16.7625$ (10) Å

$\beta = 101.266$ (3)°

$V = 4761.7$ (5) Å³

$Z = 2$

$F_{000} = 3324$

$D_x = 2.396$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2190 reflections

$\theta = 2.8$ – 27.3 °

$\mu = 2.31$ mm⁻¹

$T = 100$ K

Plates, colourless

$0.25 \times 0.15 \times 0.1$ mm

Data collection

Nonius KappaCCD
diffractometer

Radiation source: fine-focus sealed X-ray tube

Monochromator: graphite

$T = 100$ K

φ scans, and ω scans with κ offsets

Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)

$T_{\min} = 0.597$, $T_{\max} = 0.802$

45527 measured reflections

11170 independent reflections

8144 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.072$

$\theta_{\max} = 27.5$ °

$\theta_{\min} = 1.5$ °

$h = -18 \rightarrow 18$

$k = -26 \rightarrow 26$

$l = -21 \rightarrow 21$

Refinement

Refinement on F^2

Least-squares matrix: full

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$R[F^2 > 2\sigma(F^2)] = 0.036$	$w = 1/[\sigma^2(F_o^2) + (0.021P)^2]$
$wR(F^2) = 0.073$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1$	$(\Delta/\sigma)_{\max} = 0.003$
11170 reflections	$\Delta\rho_{\max} = 0.88 \text{ e } \text{\AA}^{-3}$
629 parameters	$\Delta\rho_{\min} = -0.70 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.08 (2)

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Mo1	0.56723 (3)	0.411518 (19)	0.58067 (2)	0.01535 (9)	
Mo2	0.37343 (3)	0.500847 (18)	0.56738 (2)	0.01262 (8)	
Mo5	0.41862 (3)	0.425991 (19)	0.40423 (2)	0.01562 (9)	
Mo3	0.09471 (3)	0.007942 (18)	0.90255 (2)	0.01440 (9)	
Mo4	0.12057 (3)	0.050345 (18)	1.09450 (2)	0.01550 (9)	
Mo6	-0.06607 (3)	0.102673 (18)	0.96110 (2)	0.01461 (9)	
S4	0.69926 (8)	0.32365 (5)	0.32774 (7)	0.0171 (2)	
S1	0.83864 (9)	0.32314 (6)	0.19478 (7)	0.0194 (3)	
S2	0.31973 (9)	0.32349 (5)	0.68472 (7)	0.0193 (3)	
S3	1.13888 (8)	0.41650 (5)	0.47871 (7)	0.0141 (2)	
S5	0.85700 (8)	0.41673 (5)	0.53863 (7)	0.0134 (2)	
S6	0.94719 (8)	0.41562 (5)	0.37833 (7)	0.0148 (2)	
S7	1.04691 (8)	0.41757 (5)	0.64209 (7)	0.0158 (2)	
S8	0.19893 (11)	0.75	0.39380 (10)	0.0162 (3)	
S9	0.38303 (8)	0.16665 (6)	0.03769 (7)	0.0186 (3)	
S10	-0.09582 (11)	0.75	0.43604 (10)	0.0167 (3)	
S11	0.01173 (12)	0.75	0.27956 (10)	0.0187 (4)	
S12	0.09410 (11)	0.75	0.54638 (9)	0.0157 (3)	
S13	0.57537 (8)	0.16549 (5)	0.13620 (7)	0.0169 (2)	
S14	0.47171 (8)	0.16799 (6)	-0.12637 (7)	0.0174 (2)	
S15	0.66417 (8)	0.16465 (6)	-0.02771 (7)	0.0204 (3)	
S18	0.21028 (8)	0.32348 (5)	0.83822 (7)	0.0177 (2)	
O1	0	0	1	0.0106 (9)	
O2	0.5	0.5	0.5	0.0119 (9)	
O5	0.4513 (2)	0.43340 (14)	0.62260 (17)	0.0153 (7)	
O4	0.2801 (2)	0.50318 (14)	0.61450 (18)	0.0159 (7)	
O3	0.6587 (2)	0.43007 (14)	0.51664 (18)	0.0169 (7)	

supplementary materials

O6	0.4587 (2)	0.56620 (14)	0.62598 (17)	0.0150 (7)
O12	0.4888 (2)	0.36829 (14)	0.49387 (18)	0.0161 (7)
O7	0.6179 (2)	0.49293 (14)	0.64424 (17)	0.0166 (7)
O8	-0.0228 (2)	-0.03840 (14)	0.84668 (18)	0.0195 (7)
O9	0.3326 (2)	0.44003 (14)	0.47865 (18)	0.0159 (7)
O10	0.0391 (2)	0.12578 (13)	1.03983 (18)	0.0166 (7)
O11	0.0124 (2)	0.08657 (13)	0.88356 (18)	0.0178 (7)
O13	0.1560 (2)	-0.03770 (14)	1.10491 (19)	0.0204 (7)
O14	0.1549 (2)	0.01313 (14)	0.82549 (19)	0.0215 (7)
O15	0.1685 (2)	0.05279 (13)	0.99087 (18)	0.0158 (7)
O16	0.3610 (2)	0.36980 (15)	0.33835 (19)	0.0234 (8)
O19	-0.1227 (2)	0.17476 (14)	0.93106 (19)	0.0221 (7)
O18	0.2048 (2)	0.09129 (14)	1.1612 (2)	0.0245 (8)
O17	0.6166 (2)	0.35055 (15)	0.64365 (19)	0.0245 (8)
O20	0.1308 (2)	-0.07465 (14)	0.95163 (19)	0.0200 (7)
C1	0.7991 (4)	0.25	0.2352 (4)	0.0127 (13)
C4	0.9789 (3)	0.4167 (2)	0.5449 (3)	0.0145 (9)
C3	0.1983 (5)	0.75	0.2897 (4)	0.0204 (15)
H3	0.2548	0.75	0.2703	0.025*
C2	0.7423 (4)	0.25	0.2902 (4)	0.0143 (13)
C7	0.1143 (5)	0.75	0.2388 (4)	0.0224 (15)
H7	0.1107	0.75	0.1828	0.027*
C8	0.0738 (5)	0.75	0.3820 (4)	0.0170 (14)
C6	0.8635 (3)	0.4170 (2)	0.6423 (3)	0.0166 (10)
H6	0.8088	0.4169	0.6643	0.02*
C5	0.9505 (3)	0.4174 (2)	0.6901 (3)	0.0178 (10)
H5	0.9585	0.4176	0.7465	0.021*
C11	0.2420 (4)	0.25	0.7930 (4)	0.0149 (13)
C10	0.2854 (4)	0.25	0.7292 (4)	0.0160 (14)
C15	0.5424 (3)	0.1666 (2)	-0.0301 (3)	0.0174 (10)
C16	0.5044 (3)	0.1662 (2)	0.0406 (3)	0.0172 (10)
C13	0.5655 (3)	0.1660 (2)	-0.1775 (3)	0.0216 (11)
H13	0.5553	0.166	-0.234	0.026*
C12	0.1572 (3)	0.2831 (2)	0.9098 (3)	0.0223 (11)
H12	0.1297	0.3068	0.9468	0.027*
C14	0.6539 (3)	0.1643 (2)	-0.1321 (3)	0.0210 (11)
H14	0.7074	0.163	-0.1559	0.025*
C9	0.3514 (3)	0.2832 (2)	0.6016 (3)	0.0231 (11)
H9	0.3676	0.307	0.5588	0.028*
C22	1.0177 (3)	0.41639 (19)	0.4749 (3)	0.0132 (9)
C17	0.4818 (3)	0.1637 (2)	0.1873 (3)	0.0180 (10)
H17	0.4923	0.1623	0.2438	0.022*
C18	0.3931 (3)	0.1643 (2)	0.1421 (3)	0.0185 (10)
H18	0.3396	0.1635	0.1659	0.022*
C21	0.0295 (4)	0.75	0.4457 (4)	0.0165 (14)
C20	0.6422 (3)	0.2833 (2)	0.3968 (3)	0.0211 (11)
H20	0.6127	0.307	0.4325	0.025*
C19	0.9255 (3)	0.2830 (2)	0.1533 (3)	0.0235 (11)
H19	0.9704	0.3067	0.1319	0.028*

C24	1.0417 (3)	0.4110 (2)	0.3287 (3)	0.0197 (10)	
H24	1.0322	0.4084	0.2723	0.024*	
C23	1.1297 (3)	0.4114 (2)	0.3748 (3)	0.0174 (10)	
H23	1.1836	0.4089	0.3516	0.021*	
C26	-0.0077 (4)	0.75	0.5908 (4)	0.0184 (14)	
H26	-0.0027	0.75	0.6469	0.022*	
C25	-0.0915 (5)	0.75	0.5408 (4)	0.0186 (14)	
H25	-0.1474	0.75	0.5613	0.022*	
S16	0.43075 (9)	0.99818 (6)	0.10594 (7)	0.0200 (3)	
S27	0.63331 (9)	0.99422 (6)	0.09037 (7)	0.0203 (3)	
C27	0.5135 (3)	0.9988 (2)	0.0403 (3)	0.0166 (10)	
C29	0.5178 (4)	0.9954 (2)	0.1949 (3)	0.0245 (11)	
H29	0.5008	0.9954	0.2457	0.029*	
C28	0.6083 (4)	0.9931 (2)	0.1884 (3)	0.0247 (11)	
H28	0.6568	0.991	0.2342	0.03*	
N1	0.1799 (6)	0.25	0.1110 (5)	0.061 (2)	
C30	0.1822 (6)	0.25	0.1791 (7)	0.049 (3)	
C31	0.1876 (6)	0.25	0.2689 (6)	0.050 (2)	
H31A	0.1353	0.2749	0.2815	0.076*	0.5
H31B	0.2466	0.2697	0.2953	0.076*	0.5
H31C	0.1845	0.2054	0.2876	0.076*	0.5

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.0150 (2)	0.0195 (2)	0.0125 (2)	0.00474 (16)	0.00522 (16)	0.00528 (16)
Mo2	0.01036 (18)	0.0189 (2)	0.00921 (18)	0.00057 (16)	0.00335 (15)	0.00047 (15)
Mo5	0.0138 (2)	0.0217 (2)	0.01209 (19)	-0.00355 (16)	0.00420 (16)	-0.00492 (16)
Mo3	0.0168 (2)	0.0162 (2)	0.01122 (19)	-0.00087 (16)	0.00517 (16)	0.00087 (15)
Mo4	0.0164 (2)	0.0170 (2)	0.01202 (19)	-0.00345 (16)	0.00029 (16)	-0.00233 (15)
Mo6	0.0185 (2)	0.0131 (2)	0.01240 (19)	0.00125 (16)	0.00348 (16)	0.00127 (15)
S4	0.0199 (6)	0.0162 (6)	0.0154 (6)	0.0025 (5)	0.0038 (5)	-0.0010 (5)
S1	0.0213 (6)	0.0191 (6)	0.0189 (6)	-0.0011 (5)	0.0062 (5)	0.0029 (5)
S2	0.0241 (7)	0.0177 (6)	0.0166 (6)	-0.0050 (5)	0.0055 (5)	0.0010 (5)
S3	0.0110 (5)	0.0164 (6)	0.0148 (6)	-0.0019 (4)	0.0023 (5)	-0.0003 (4)
S5	0.0114 (5)	0.0163 (6)	0.0122 (5)	0.0001 (4)	0.0018 (4)	0.0009 (4)
S6	0.0148 (6)	0.0171 (6)	0.0117 (5)	-0.0021 (4)	0.0006 (5)	0.0014 (4)
S7	0.0152 (6)	0.0186 (6)	0.0121 (5)	-0.0005 (5)	-0.0008 (5)	0.0000 (4)
S8	0.0155 (8)	0.0175 (8)	0.0151 (8)	0	0.0017 (7)	0
S9	0.0149 (6)	0.0223 (6)	0.0184 (6)	-0.0005 (5)	0.0028 (5)	-0.0022 (5)
S10	0.0151 (8)	0.0176 (8)	0.0161 (8)	0	-0.0006 (7)	0
S11	0.0227 (9)	0.0184 (8)	0.0124 (8)	0	-0.0027 (7)	0
S12	0.0155 (8)	0.0173 (8)	0.0126 (8)	0	-0.0016 (7)	0
S13	0.0163 (6)	0.0215 (6)	0.0127 (6)	0.0001 (5)	0.0021 (5)	-0.0004 (5)
S14	0.0188 (6)	0.0213 (6)	0.0118 (6)	0.0011 (5)	0.0019 (5)	-0.0001 (5)
S15	0.0158 (6)	0.0278 (7)	0.0182 (6)	0.0030 (5)	0.0046 (5)	0.0017 (5)
S18	0.0210 (6)	0.0147 (6)	0.0177 (6)	-0.0002 (5)	0.0046 (5)	-0.0021 (5)
O1	0.013 (2)	0.012 (2)	0.007 (2)	-0.0012 (17)	0.0024 (17)	-0.0010 (16)

supplementary materials

O2	0.010 (2)	0.016 (2)	0.011 (2)	0.0002 (17)	0.0043 (18)	0.0001 (17)
O5	0.0175 (17)	0.0193 (16)	0.0103 (15)	0.0010 (13)	0.0054 (13)	0.0021 (12)
O4	0.0135 (16)	0.0218 (17)	0.0133 (16)	-0.0001 (13)	0.0047 (13)	-0.0004 (13)
O3	0.0134 (16)	0.0221 (16)	0.0164 (17)	0.0041 (13)	0.0052 (14)	0.0028 (13)
O6	0.0153 (16)	0.0199 (16)	0.0109 (15)	-0.0017 (13)	0.0053 (13)	-0.0024 (13)
O12	0.0207 (17)	0.0149 (16)	0.0149 (16)	-0.0004 (13)	0.0091 (14)	-0.0004 (12)
O7	0.0131 (16)	0.0259 (17)	0.0102 (16)	0.0016 (13)	0.0012 (13)	0.0014 (13)
O8	0.0240 (18)	0.0230 (17)	0.0114 (16)	-0.0007 (14)	0.0032 (14)	-0.0036 (13)
O9	0.0137 (16)	0.0207 (17)	0.0149 (16)	-0.0036 (13)	0.0068 (13)	-0.0031 (13)
O10	0.0193 (17)	0.0122 (15)	0.0188 (17)	-0.0036 (13)	0.0049 (14)	-0.0019 (13)
O11	0.0200 (17)	0.0164 (16)	0.0168 (17)	-0.0021 (13)	0.0026 (14)	0.0020 (13)
O13	0.0192 (17)	0.0219 (17)	0.0173 (17)	-0.0010 (14)	-0.0034 (14)	0.0015 (14)
O14	0.0254 (19)	0.0192 (17)	0.0229 (19)	-0.0013 (14)	0.0120 (16)	0.0011 (14)
O15	0.0126 (16)	0.0171 (16)	0.0183 (17)	-0.0035 (13)	0.0040 (13)	-0.0032 (13)
O16	0.0220 (18)	0.0321 (19)	0.0167 (18)	-0.0051 (15)	0.0054 (15)	-0.0125 (14)
O19	0.0264 (19)	0.0181 (17)	0.0227 (18)	0.0025 (14)	0.0066 (16)	0.0043 (14)
O18	0.0244 (18)	0.0251 (18)	0.0215 (18)	-0.0084 (14)	-0.0017 (15)	-0.0043 (14)
O17	0.028 (2)	0.0275 (18)	0.0197 (19)	0.0115 (15)	0.0097 (16)	0.0075 (14)
O20	0.0219 (18)	0.0160 (16)	0.0245 (19)	-0.0015 (13)	0.0102 (15)	-0.0005 (14)
C1	0.015 (3)	0.013 (3)	0.011 (3)	0	0.006 (3)	0
C4	0.011 (2)	0.012 (2)	0.019 (2)	0.0005 (17)	-0.0005 (19)	0.0019 (18)
C3	0.022 (4)	0.028 (4)	0.012 (3)	0	0.006 (3)	0
C2	0.018 (3)	0.014 (3)	0.009 (3)	0	-0.002 (3)	0
C7	0.036 (4)	0.021 (4)	0.012 (3)	0	0.010 (3)	0
C8	0.026 (4)	0.019 (3)	0.005 (3)	0	-0.001 (3)	0
C6	0.016 (2)	0.017 (2)	0.018 (2)	0.0003 (18)	0.006 (2)	0.0009 (19)
C5	0.026 (3)	0.017 (2)	0.011 (2)	-0.002 (2)	0.005 (2)	-0.0006 (18)
C11	0.014 (3)	0.015 (3)	0.014 (3)	0	-0.003 (3)	0
C10	0.016 (3)	0.015 (3)	0.015 (3)	0	0.000 (3)	0
C15	0.016 (2)	0.021 (2)	0.014 (2)	0.0026 (19)	0.001 (2)	-0.0020 (19)
C16	0.019 (2)	0.018 (2)	0.015 (2)	-0.0004 (19)	0.004 (2)	-0.0005 (19)
C13	0.032 (3)	0.021 (3)	0.014 (2)	0.005 (2)	0.010 (2)	0.0023 (19)
C12	0.019 (3)	0.028 (3)	0.021 (3)	0.005 (2)	0.009 (2)	-0.001 (2)
C14	0.020 (3)	0.028 (3)	0.017 (3)	0.006 (2)	0.010 (2)	0.001 (2)
C9	0.024 (3)	0.031 (3)	0.016 (3)	-0.003 (2)	0.008 (2)	0.002 (2)
C22	0.014 (2)	0.007 (2)	0.016 (2)	-0.0029 (17)	-0.0017 (19)	-0.0001 (17)
C17	0.023 (3)	0.019 (2)	0.013 (2)	0.001 (2)	0.007 (2)	-0.0021 (19)
C18	0.021 (3)	0.016 (2)	0.022 (3)	-0.0033 (19)	0.011 (2)	-0.0040 (19)
C21	0.014 (3)	0.018 (3)	0.013 (3)	0	-0.006 (3)	0
C20	0.024 (3)	0.030 (3)	0.010 (2)	0.006 (2)	0.007 (2)	-0.0007 (19)
C19	0.023 (3)	0.034 (3)	0.017 (3)	-0.003 (2)	0.011 (2)	0.001 (2)
C24	0.025 (3)	0.022 (3)	0.011 (2)	-0.005 (2)	0.002 (2)	0.0009 (19)
C23	0.021 (2)	0.020 (2)	0.012 (2)	-0.0021 (19)	0.005 (2)	0.0018 (18)
C26	0.021 (4)	0.015 (3)	0.020 (4)	0	0.005 (3)	0
C25	0.027 (4)	0.013 (3)	0.017 (3)	0	0.006 (3)	0
S16	0.0263 (7)	0.0219 (6)	0.0124 (6)	0.0039 (5)	0.0053 (5)	-0.0005 (5)
S27	0.0219 (6)	0.0245 (6)	0.0127 (6)	0.0035 (5)	-0.0012 (5)	-0.0004 (5)
C27	0.021 (2)	0.015 (2)	0.013 (2)	0.0028 (19)	0.003 (2)	-0.0002 (18)
C29	0.039 (3)	0.022 (3)	0.010 (2)	0.002 (2)	-0.001 (2)	-0.0004 (19)

C28	0.035 (3)	0.022 (3)	0.012 (2)	0.005 (2)	-0.007 (2)	-0.0015 (19)
N1	0.071 (6)	0.060 (5)	0.050 (5)	0	0.002 (5)	0
C30	0.038 (5)	0.026 (5)	0.084 (8)	0	0.014 (6)	0
C31	0.051 (6)	0.033 (5)	0.071 (7)	0	0.021 (5)	0

Geometric parameters (Å, °)

Mo1—O17	1.686 (3)	S15—C14	1.727 (5)
Mo1—O12	1.872 (3)	S15—C15	1.736 (5)
Mo1—O3	1.886 (3)	S18—C12	1.743 (5)
Mo1—O5	1.974 (3)	S18—C11	1.768 (4)
Mo1—O7	2.018 (3)	O1—Mo6 ⁱⁱ	2.3222 (4)
Mo1—O2	2.3345 (4)	O1—Mo3 ⁱⁱ	2.3234 (4)
Mo2—O4	1.680 (3)	O1—Mo4 ⁱⁱ	2.3363 (4)
Mo2—O5	1.887 (3)	O2—Mo2 ⁱ	2.3151 (4)
Mo2—O9	1.931 (3)	O2—Mo5 ⁱ	2.3335 (4)
Mo2—O6	1.932 (3)	O2—Mo1 ⁱ	2.3345 (4)
Mo2—O3 ⁱ	1.974 (3)	O3—Mo2 ⁱ	1.974 (3)
Mo2—O2	2.3151 (4)	O6—Mo5 ⁱ	1.928 (3)
Mo5—O16	1.684 (3)	O7—Mo5 ⁱ	1.860 (3)
Mo5—O7 ⁱ	1.860 (3)	O8—Mo4 ⁱⁱ	1.879 (3)
Mo5—O6 ⁱ	1.928 (3)	O13—Mo6 ⁱⁱ	2.013 (3)
Mo5—O9	1.937 (3)	O20—Mo6 ⁱⁱ	1.962 (3)
Mo5—O12	2.010 (3)	C1—C2	1.343 (8)
Mo5—O2	2.3335 (4)	C1—S1 ⁱⁱⁱ	1.766 (3)
Mo3—O14	1.690 (3)	C4—C22	1.393 (6)
Mo3—O15	1.876 (3)	C3—C7	1.331 (9)
Mo3—O20	1.889 (3)	C3—H3	0.93
Mo3—O11	1.968 (3)	C2—S4 ⁱⁱⁱ	1.774 (4)
Mo3—O8	1.993 (3)	C7—H7	0.93
Mo3—O1	2.3234 (4)	C8—C21	1.345 (9)
Mo4—O18	1.692 (3)	C6—C5	1.343 (6)
Mo4—O13	1.851 (3)	C6—H6	0.93
Mo4—O8 ⁱⁱ	1.879 (3)	C5—H5	0.93
Mo4—O15	1.989 (3)	C11—C10	1.339 (9)
Mo4—O10	2.028 (3)	C11—S18 ⁱⁱⁱ	1.768 (4)
Mo4—O1	2.3363 (4)	C10—S2 ⁱⁱⁱ	1.774 (4)
Mo6—O19	1.696 (3)	C15—C16	1.398 (6)
Mo6—O10	1.858 (3)	C13—C14	1.343 (6)
Mo6—O11	1.905 (3)	C13—H13	0.93
Mo6—O20 ⁱⁱ	1.962 (3)	C12—C12 ⁱⁱⁱ	1.340 (9)
Mo6—O13 ⁱⁱ	2.013 (3)	C12—H12	0.93
Mo6—O1	2.3222 (4)	C14—H14	0.93
S4—C20	1.746 (5)	C9—C9 ⁱⁱⁱ	1.343 (9)
S4—C2	1.774 (4)	C9—H9	0.93

supplementary materials

S1—C19	1.739 (5)	C17—C18	1.347 (6)
S1—C1	1.766 (3)	C17—H17	0.93
S2—C9	1.749 (5)	C18—H18	0.93
S2—C10	1.774 (4)	C20—C20 ⁱⁱⁱ	1.347 (9)
S3—C23	1.723 (4)	C20—H20	0.93
S3—C22	1.724 (4)	C19—C19 ⁱⁱⁱ	1.335 (9)
S5—C6	1.721 (5)	C19—H19	0.93
S5—C4	1.727 (4)	C24—C23	1.344 (6)
S6—C24	1.724 (5)	C24—H24	0.93
S6—C22	1.732 (4)	C23—H23	0.93
S7—C4	1.728 (4)	C26—C25	1.323 (9)
S7—C5	1.728 (5)	C26—H26	0.93
S8—C3	1.743 (6)	C25—H25	0.93
S8—C8	1.764 (7)	S16—C29	1.748 (5)
S9—C18	1.728 (5)	S16—C27	1.767 (5)
S9—C16	1.728 (5)	S27—C28	1.749 (5)
S10—C25	1.746 (6)	S27—C27	1.759 (5)
S10—C21	1.769 (6)	C27—C27 ^{iv}	1.330 (8)
S11—C7	1.737 (7)	C29—C28	1.322 (7)
S11—C8	1.772 (6)	C29—H29	0.93
S12—C21	1.759 (6)	C28—H28	0.93
S12—C26	1.761 (7)	N1—C30	1.136 (12)
S13—C16	1.722 (5)	C30—C31	1.492 (13)
S13—C17	1.725 (5)	C31—H31A	0.96
S14—C15	1.729 (4)	C31—H31B	0.96
S14—C13	1.729 (5)	C31—H31C	0.96
O17—Mo1—O12	105.04 (14)	Mo2—O2—Mo5 ⁱ	89.589 (13)
O17—Mo1—O3	104.43 (14)	Mo2 ⁱ —O2—Mo5 ⁱ	90.411 (14)
O12—Mo1—O3	91.61 (13)	Mo2—O2—Mo5	90.411 (14)
O17—Mo1—O5	102.70 (14)	Mo2 ⁱ —O2—Mo5	89.589 (13)
O12—Mo1—O5	87.90 (12)	Mo5 ⁱ —O2—Mo5	180.000 (15)
O3—Mo1—O5	152.02 (12)	Mo2—O2—Mo1	89.800 (13)
O17—Mo1—O7	101.69 (14)	Mo2 ⁱ —O2—Mo1	90.200 (13)
O12—Mo1—O7	152.99 (12)	Mo5 ⁱ —O2—Mo1	89.969 (14)
O3—Mo1—O7	85.42 (12)	Mo5—O2—Mo1	90.031 (14)
O5—Mo1—O7	82.51 (12)	Mo2—O2—Mo1 ⁱ	90.200 (13)
O17—Mo1—O2	176.68 (11)	Mo2 ⁱ —O2—Mo1 ⁱ	89.800 (13)
O12—Mo1—O2	77.94 (9)	Mo5 ⁱ —O2—Mo1 ⁱ	90.031 (14)
O3—Mo1—O2	76.77 (9)	Mo5—O2—Mo1 ⁱ	89.969 (14)
O5—Mo1—O2	75.78 (8)	Mo1—O2—Mo1 ⁱ	180
O7—Mo1—O2	75.24 (8)	Mo2—O5—Mo1	116.42 (14)
O4—Mo2—O5	103.76 (13)	Mo1—O3—Mo2 ⁱ	117.16 (14)
O4—Mo2—O9	103.37 (13)	Mo5 ⁱ —O6—Mo2	116.11 (14)
O5—Mo2—O9	88.74 (12)	Mo1—O12—Mo5	116.50 (14)
O4—Mo2—O6	102.89 (13)	Mo5 ⁱ —O7—Mo1	116.59 (14)

O5—Mo2—O6	89.50 (12)	Mo4 ⁱⁱ —O8—Mo3	117.46 (15)
O9—Mo2—O6	153.33 (12)	Mo2—O9—Mo5	117.05 (14)
O4—Mo2—O3 ⁱ	102.71 (13)	Mo6—O10—Mo4	116.53 (14)
O5—Mo2—O3 ⁱ	153.52 (12)	Mo6—O11—Mo3	116.24 (15)
O9—Mo2—O3 ⁱ	84.73 (12)	Mo4—O13—Mo6 ⁱⁱ	116.26 (15)
O6—Mo2—O3 ⁱ	85.07 (12)	Mo3—O15—Mo4	116.10 (14)
O4—Mo2—O2	178.36 (10)	Mo3—O20—Mo6 ⁱⁱ	116.81 (15)
O5—Mo2—O2	77.87 (9)	C2—C1—S1	123.08 (17)
O9—Mo2—O2	76.54 (9)	C2—C1—S1 ⁱⁱⁱ	123.08 (17)
O6—Mo2—O2	77.07 (9)	S1—C1—S1 ⁱⁱⁱ	113.8 (3)
O3 ⁱ —Mo2—O2	75.66 (8)	C22—C4—S5	120.9 (3)
O16—Mo5—O7 ⁱ	104.41 (14)	C22—C4—S7	123.4 (3)
O16—Mo5—O6 ⁱ	103.77 (14)	S5—C4—S7	115.7 (3)
O7 ⁱ —Mo5—O6 ⁱ	90.34 (12)	C7—C3—S8	118.0 (5)
O16—Mo5—O9	103.27 (14)	C7—C3—H3	121
O7 ⁱ —Mo5—O9	89.55 (12)	S8—C3—H3	121
O6 ⁱ —Mo5—O9	152.09 (12)	C1—C2—S4 ⁱⁱⁱ	122.83 (18)
O16—Mo5—O12	101.98 (14)	C1—C2—S4	122.83 (18)
O7 ⁱ —Mo5—O12	153.60 (12)	S4 ⁱⁱⁱ —C2—S4	114.3 (4)
O6 ⁱ —Mo5—O12	84.01 (12)	C3—C7—S11	118.3 (5)
O9—Mo5—O12	83.78 (12)	C3—C7—H7	120.8
O16—Mo5—O2	177.36 (11)	S11—C7—H7	120.8
O7 ⁱ —Mo5—O2	78.16 (9)	C21—C8—S8	122.5 (5)
O6 ⁱ —Mo5—O2	76.70 (8)	C21—C8—S11	123.0 (5)
O9—Mo5—O2	75.98 (8)	S8—C8—S11	114.5 (4)
O12—Mo5—O2	75.45 (8)	C5—C6—S5	117.6 (4)
O14—Mo3—O15	106.28 (14)	C5—C6—H6	121.2
O14—Mo3—O20	104.51 (14)	S5—C6—H6	121.2
O15—Mo3—O20	91.14 (13)	C6—C5—S7	117.0 (4)
O14—Mo3—O11	101.82 (14)	C6—C5—H5	121.5
O15—Mo3—O11	87.94 (12)	S7—C5—H5	121.5
O20—Mo3—O11	152.81 (13)	C10—C11—S18 ⁱⁱⁱ	122.77 (18)
O14—Mo3—O8	100.35 (14)	C10—C11—S18	122.77 (18)
O15—Mo3—O8	153.12 (13)	S18 ⁱⁱⁱ —C11—S18	114.5 (4)
O20—Mo3—O8	85.58 (13)	C11—C10—S2	123.05 (18)
O11—Mo3—O8	83.12 (12)	C11—C10—S2 ⁱⁱⁱ	123.05 (18)
O14—Mo3—O1	175.05 (11)	S2—C10—S2 ⁱⁱⁱ	113.8 (4)
O15—Mo3—O1	78.15 (9)	C16—C15—S14	122.5 (3)
O20—Mo3—O1	77.32 (9)	C16—C15—S15	122.4 (3)
O11—Mo3—O1	75.90 (9)	S14—C15—S15	115.1 (3)
O8—Mo3—O1	75.10 (9)	C15—C16—S13	122.1 (4)
O18—Mo4—O13	105.18 (14)	C15—C16—S9	122.2 (4)
O18—Mo4—O8 ⁱⁱ	102.97 (15)	S13—C16—S9	115.7 (3)
O13—Mo4—O8 ⁱⁱ	92.59 (13)	C14—C13—S14	117.2 (4)

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O18—Mo4—O15	103.98 (14)	C14—C13—H13	121.4
O13—Mo4—O15	88.36 (13)	S14—C13—H13	121.4
O8 ⁱⁱ —Mo4—O15	151.77 (12)	C12 ⁱⁱⁱ —C12—S18	117.92 (15)
O18—Mo4—O10	101.72 (13)	C12 ⁱⁱⁱ —C12—H12	121
O13—Mo4—O10	152.84 (12)	S18—C12—H12	121
O8 ⁱⁱ —Mo4—O10	84.97 (12)	C13—C14—S15	117.2 (4)
O15—Mo4—O10	81.52 (12)	C13—C14—H14	121.4
O18—Mo4—O1	176.53 (11)	S15—C14—H14	121.4
O13—Mo4—O1	78.29 (9)	C9 ⁱⁱⁱ —C9—S2	117.77 (15)
O8 ⁱⁱ —Mo4—O1	76.83 (9)	C9 ⁱⁱⁱ —C9—H9	121.1
O15—Mo4—O1	75.75 (8)	S2—C9—H9	121.1
O10—Mo4—O1	74.81 (8)	C4—C22—S3	122.2 (3)
O19—Mo6—O10	105.57 (14)	C4—C22—S6	122.1 (3)
O19—Mo6—O11	104.81 (14)	S3—C22—S6	115.7 (3)
O10—Mo6—O11	91.35 (13)	C18—C17—S13	117.3 (4)
O19—Mo6—O20 ⁱⁱ	101.65 (14)	C18—C17—H17	121.3
O10—Mo6—O20 ⁱⁱ	88.78 (13)	S13—C17—H17	121.3
O11—Mo6—O20 ⁱⁱ	152.48 (12)	C17—C18—S9	117.0 (4)
O19—Mo6—O13 ⁱⁱ	100.43 (14)	C17—C18—H18	121.5
O10—Mo6—O13 ⁱⁱ	153.81 (12)	S9—C18—H18	121.5
O11—Mo6—O13 ⁱⁱ	84.97 (13)	C8—C21—S12	121.4 (5)
O20 ⁱⁱ —Mo6—O13 ⁱⁱ	82.91 (13)	C8—C21—S10	123.7 (5)
O19—Mo6—O1	175.58 (11)	S12—C21—S10	115.0 (4)
O10—Mo6—O1	78.25 (9)	C20 ⁱⁱⁱ —C20—S4	117.88 (15)
O11—Mo6—O1	77.08 (8)	C20 ⁱⁱⁱ —C20—H20	121.1
O20 ⁱⁱ —Mo6—O1	76.01 (9)	S4—C20—H20	121.1
O13 ⁱⁱ —Mo6—O1	75.65 (8)	C19 ⁱⁱⁱ —C19—S1	117.84 (15)
C20—S4—C2	94.7 (2)	C19 ⁱⁱⁱ —C19—H19	121.1
C19—S1—C1	94.0 (2)	S1—C19—H19	121.1
C9—S2—C10	94.6 (2)	C23—C24—S6	117.3 (4)
C23—S3—C22	94.9 (2)	C23—C24—H24	121.4
C6—S5—C4	94.8 (2)	S6—C24—H24	121.4
C24—S6—C22	94.7 (2)	C24—C23—S3	117.4 (4)
C4—S7—C5	94.9 (2)	C24—C23—H23	121.3
C3—S8—C8	94.6 (3)	S3—C23—H23	121.3
C18—S9—C16	95.0 (2)	C25—C26—S12	117.1 (5)
C25—S10—C21	94.1 (3)	C25—C26—H26	121.4
C7—S11—C8	94.5 (3)	S12—C26—H26	121.4
C21—S12—C26	94.7 (3)	C26—C25—S10	119.1 (5)
C16—S13—C17	95.0 (2)	C26—C25—H25	120.4
C15—S14—C13	95.3 (2)	S10—C25—H25	120.4
C14—S15—C15	95.2 (2)	C29—S16—C27	94.5 (2)
C12—S18—C11	94.8 (2)	C28—S27—C27	95.1 (2)
Mo6—O1—Mo6 ⁱⁱ	180.000 (19)	C27 ^{iv} —C27—S27	123.3 (5)
Mo6—O1—Mo3 ⁱⁱ	89.861 (13)	C27 ^{iv} —C27—S16	122.4 (5)

Mo6 ⁱⁱ —O1—Mo3 ⁱⁱ	90.139 (13)	S27—C27—S16	114.3 (2)
Mo6—O1—Mo3	90.139 (13)	C28—C29—S16	118.5 (4)
Mo6 ⁱⁱ —O1—Mo3	89.861 (13)	C28—C29—H29	120.8
Mo3 ⁱⁱ —O1—Mo3	180.0000 (10)	S16—C29—H29	120.8
Mo6—O1—Mo4	90.402 (14)	C29—C28—S27	117.5 (4)
Mo6 ⁱⁱ —O1—Mo4	89.598 (13)	C29—C28—H28	121.3
Mo3 ⁱⁱ —O1—Mo4	90.504 (14)	S27—C28—H28	121.3
Mo3—O1—Mo4	89.496 (14)	N1—C30—C31	178.7 (11)
Mo6—O1—Mo4 ⁱⁱ	89.598 (13)	C30—C31—H31A	109.5
Mo6 ⁱⁱ —O1—Mo4 ⁱⁱ	90.402 (14)	C30—C31—H31B	109.5
Mo3 ⁱⁱ —O1—Mo4 ⁱⁱ	89.496 (14)	H31A—C31—H31B	109.5
Mo3—O1—Mo4 ⁱⁱ	90.504 (14)	C30—C31—H31C	109.5
Mo4—O1—Mo4 ⁱⁱ	180.0000 (10)	H31A—C31—H31C	109.5
Mo2—O2—Mo2 ⁱ	180	H31B—C31—H31C	109.5

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C5—H5 \cdots O11 ^v	0.93	2.28	3.192 (6)	167
C7—H7 \cdots O19 ^{vi}	0.93	2.47	3.251 (7)	141
C7—H7 \cdots O19 ^{vii}	0.93	2.47	3.251 (7)	141
C9—H9 \cdots O12	0.93	2.54	3.388 (5)	151
C13—H13 \cdots O17 ^{viii}	0.93	2.41	3.239 (6)	149
C14—H14 \cdots O19 ^{ix}	0.93	2.59	3.175 (5)	121
C18—H18 \cdots O18 ^x	0.93	2.41	3.145 (5)	136
C19—H19 \cdots O10 ^{xi}	0.93	2.41	3.298 (5)	160
C20—H20 \cdots O12	0.93	2.54	3.437 (5)	162
C24—H24 \cdots O8 ^{xii}	0.93	2.25	3.075 (6)	148
C28—H28 \cdots O4 ^{xii}	0.93	2.53	3.384 (6)	152
C29—H29 \cdots O5 ^{xii}	0.93	2.52	3.256 (6)	137
C29—H29 \cdots O6 ^{xii}	0.93	2.55	3.284 (6)	136

Symmetry codes: (v) $x+1, -y+1/2, z$; (vi) $-x, y+1/2, -z+1$; (vii) $-x, -y+1, -z+1$; (viii) $x, -y+1/2, z-1$; (ix) $x+1, y, z-1$; (x) $x, y, z-1$; (xi) $x+1, -y+1/2, z-1$; (xii) $-x+1, y+1/2, -z+1$.

Fig. 1

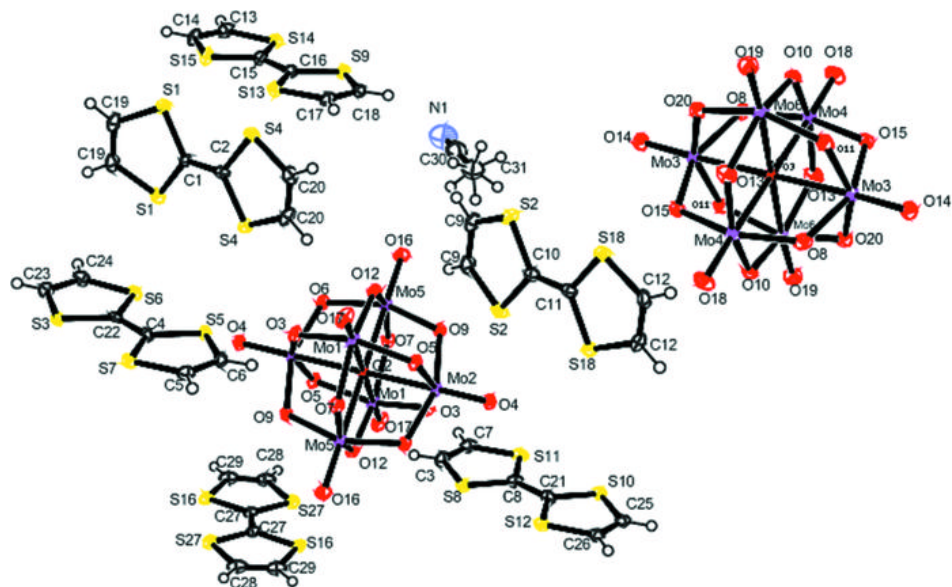


Fig. 2

