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1-(1*H*-1,3-Benzimidazol-2-yl)guanidinium dihydrogendodecamolybdophosphate–methanol–water (1/2.5/4)

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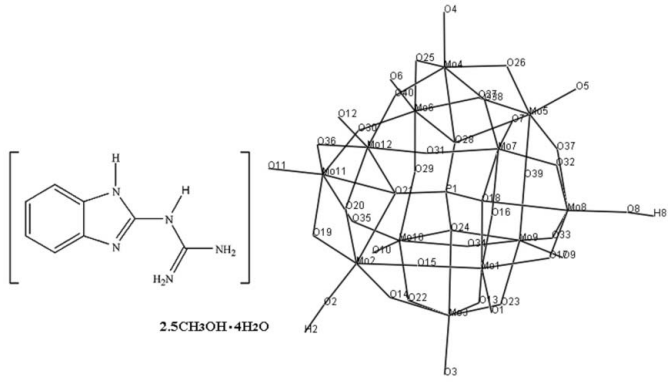
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.018 Å; disorder in solvent or counterion; R factor = 0.043; wR factor = 0.095; data-to-parameter ratio = 15.0.

The three-dimensional supramolecular aggregation in the title hybrid material, $(C_8H_{10}N_5)[H_2PMo_{12}O_{40}]\cdot2.5CH_3OH\cdot4H_2O$, is based on the formation of O—H···O, N—H···O and O—H···N hydrogen bonds, and O···O and N···O electrostatic interactions (O···O = 2.95–3.04 Å and N···O = 2.91–3.01 Å). Water and methanol solvent molecules make infinite zigzag belts around the organic cations and Keggin polyoxoanions with a chain sequence $H_2O\cdots CH_3OH\cdots CH_3OH\cdots CH_3OH\cdots H_2O\cdots H_2O\cdots CH_3OH\cdots$. Each symmetry-unique water and methanol molecule forms distinct interactions with the other components in the crystal structure. Five methanol solvent molecules in the crystal lattice have site-occupancy factors of 0.5.

Related literature

For related literature, see: Andrade-López *et al.* (1997); Batsanov *et al.* (2006); Corbridge (1995); Coronado & Gómez-García (1998); Coronado *et al.* (2004); Du *et al.* (2005); Duarte *et al.* (2005); Gholivand *et al.* (2006); King *et al.* (1948); Laberge (1998); Li *et al.* (2005); Liu *et al.* (2004); Ma *et al.* (2005); Madhu & Das (2004); Meot-Ner (2005); Santos *et al.* (2005); Steel (1991); Tan *et al.* (2005); Zhang *et al.* (1997).



Experimental

Crystal data

$(C_8H_{10}N_5)[H_2PMo_{12}O_{40}]\cdot2.5CH_4O\cdot4H_2O$
M_r = 2152.65
Monoclinic, $P2_1$
a = 11.9025 (12) Å
b = 18.2497 (19) Å
c = 12.7798 (13) Å
β = 109.639 (2)°
V = 2614.5 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 2.92 mm^{-1}
T = 120 (2) K
0.40 × 0.30 × 0.15 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi scan (*SADABS*; Sheldrick, 1998*a*)
T_{min} = 0.360, T_{max} = 0.648
22667 measured reflections
9960 independent reflections
9679 reflections with $I > 2\sigma(I)$
R_{int} = 0.093

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.095
S = 1.05
9960 reflections
663 parameters
30 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.68 e Å^{-3}
$\Delta\rho_{min}$ = −1.28 e Å^{-3}
Absolute structure: Flack (1983), 4793 Friedel pairs
Flack parameter: 0.04 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O4^{i}	0.96	2.14	3.097 (9)	173
O8—H8···O10^{ii}	0.96	2.40	3.093 (5)	129
N1—H1N1···O5S^{iii}	0.88	1.95	2.728 (6)	146
N1—H2N1···O5W^{iv}	0.88	2.20	2.883 (6)	134
N2—H1N2···O5S^{iii}	0.88	2.10	2.839 (6)	141
N2—H2N2···O5	0.88	2.01	2.844 (6)	157
N3—H1N3···O1W	0.90	1.84	2.717 (6)	165
N5—H1N5···O36^{ii}	0.90	2.25	2.974 (5)	137
O1S—H1OS···O32	0.95	2.35	3.218 (5)	152
O3S—H3OS···O5W^{v}	0.96	2.01	2.881 (7)	149
O4S—H4OS···O27	0.96	1.99	2.805 (6)	141
O1W—H1W1···O20^{ii}	1.01	1.89	2.740 (6)	140
O1W—H2W1···O5W'^{iv}	1.01	2.05	3.057 (7)	176
O1W—H2W1···O5W^{iv}	1.01	2.17	3.067 (7)	148
O2W—H2W2···N4	1.01	1.78	2.731 (6)	157
O3W—H2W3···O3S	1.01	1.93	2.618 (8)	123
O4W—H1W4···O6^{ii}	1.01	2.30	3.004 (7)	126
O4W—H2W4···O2S	1.01	1.76	2.716 (7)	157
O5W—H4W'···O32^{vi}	1.01	1.87	2.847 (7)	161

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

  doi:10.1107/S1600536807046612

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 1998); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998*b*); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: LH2487).

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supplementary materials

Acta Cryst. (2007). E**63**, m2622-m2623 [**doi:10.1107/S1600536807046612**]

1-(1*H*-1,3-Benzimidazol-2-yl)guanidinium dihydrogendodecamolybdophosphate-methanol-water (1/2.5/4)

M. Pourayoubi and A. R. Mahjoub

Comment

Non-covalent forces play a vital role in crystal packing (Du *et al.*, 2005) which are important for material sciences, supramolecular chemistry and biology (Tan *et al.*, 2005; Duarte *et al.*, 2005; Li *et al.*, 2005; Meot-Ner, 2005; Madhu & Das, 2004; Laberge, 1998). In this subject, some discussions carried out on the electrostatic interactions (Liu *et al.*, 2004), symmetrical aspects and the hydrogen bonds functions (Gholivand, *et al.*, 2006). Hence, we study these interactions in a new polyoxometalate (POM)-based organic/inorganic hybrid containing a polyfunctional molecule 2-gb [*N*-(1*H*-1,3-benzimidazol-2-yl)guanidine (2-guanidinobenzimidazole)] as the organic component. Due to the importance of crystal engineering in material studies (Batsanov *et al.*, 2006) and the value of material hybrids based on the polyoxometalates, POMs, (Santos, *et al.*, 2005; Ma, *et al.*, 2005; Coronado, *et al.*, 2004; Coronado & Gómez-García, 1998; Zhang, *et al.*, 1997) this investigation may be useful. The basic unit of title hybrid contains asymmetric $[H_2PMo_{12}O_{40}]^-$ polyoxoanion (Fig. 1) and 2-gbH$^+$ cation (Fig. 2) besides the solvated H_2O and CH_3OH molecules (5 CH_3OH molecules with the site occupancy factor of 0.5 and 4 H_2O). Four different kinds of O atoms occur in bifunctional Keggin acid: a) the 12 terminal, b) the 4 bonded to P and Mo, c) the 12 Mo_O6 octahedra corner-shared and d) the 12 MoO_6 octahedra edge-shared. The phosphorus atom has a tetrahedral configuration (O—P—O angles in the range of 109.1 (3)°-109.9 (3)°) and the Mo atoms are distorted octahedral (152.9 (3)°-170.4 (3)° for *trans* O—Mo—O angles). The P—O bonds are in the range of P—O single bond (Corbridge, 1995), 1.531 (6)–1.550 (6) Å. Five N atoms are in 2-gb and only one is protonatated (guanidine N(3) atom) to form a $C_8H_{10}N_5^+$ cation, like previous study on [2-gbH]$^+$ACO$^-$·H_2O (Andrade-López, *et al.*, 1997). The C(1)—N(1), C(1)—N(2) and C(1)—N(3) bonds, consistent with the guanidine functional group, are not equivalent in title compound. C(1)—N(1) and C(1)—N(2) bond distances are in the range of "one-and a half bonds" which are strengthened *versus* to these bonds in free ligand (1.311 (13) Å, 1.326 (12) Å in compare with the 1.350 (4) Å and 1.357 (4) Å (Steel, 1991). This is attributed to contribution of nitrogen atoms lone pair in C(1)—N(1) and C(1)—N(2) bonds. This effect causes that the angle N(1)—C(1)—N(2) become greater in the title compound with compare to the corresponding angle in free ligand (121.5 (9) and 117.7 (3)°). C(1)—N(3) is a single bond in POM-based organic/inorganic hybrid, 1.374 (13) Å (*versus* 1.321 (4) Å in free ligand). In 2-gbH$^+$ cation, the guanidinium residue is twisted from the nearly planar benzimidazole moiety (torsion angles C(1)—N(3)—C(2)—N(4) and C(1)—N(3)—C(2)—N(5) are 38.3 (15)° and −149.1 (9)°, respectively. Various O—H···O and N—H···O hydrogen bonds (Table 1) in the crystal lattice (and also different O···O and N···O electrostatic interactions) lead to a 3-D supramolecular framework. Via the five nitrogen atoms, 2-gbH$^+$ cation is surrounded by three $[H_2PMo_{12}O_{40}]^-$ anions (with two N—H···O hydrogen bonds and one electrostatic interaction), and three H_2O molecules. Figure 3 shows the location of organic cation between three inorganic anions which the interaction of 2-gbH$^+$ with the left anion in figure is an electrostatic interaction. N(2) and N(5) atoms of 2-gbH$^+$ are hydrogen bonded to terminal O(5) and edge-shared O(36) atoms of POMs (N(2)···O(5) = 2.844 (6) Å and (N(5)···O(36) = 2.974 (5) Å). Besides the solvated CH_3OH and H_2O molecules, the anion is connected to 3 other neighboring anions *via* the O···O electrostatic interactions and three 2-gbH$^+$ cations (*via* N···O electrostatic interactions and two N—H···O hydrogen bonds, N(2)—H(2 N2)···O(5) and N(5)—H(1 N5)···O(36). Crystal

packing of polyoxoanions and view of the unit cell packing along *b* crystal axis are shown in Figs. 4 and 5. Some H_2O and CH_3OH solvated molecules make infinite zigzag belts around the organic cations and the inorganic anions with the sequence of $H_2O\cdots CH_3OH\cdots CH_3OH\cdots CH_3OH\cdots H_2O\cdots H_2O\cdots CH_3OH\cdots$ in the chains (Fig. 6). All solvated H_2O (as well as CH_3OH) molecules are symmetrically non-equivalent in case of their various interactions with the other components in crystal lattice.

Experimental

2-Gb was prepared by the cyclocondensation of cyanoguanidine and *o*-phenylenediamine according to the method reported by King and co-worker (King, *et al.*, 1948). Synthesis of $[2\text{-gbH}][H_2PMo_{12}O_{40}]\cdot 2.5CH_3OH\cdot 4H_2O$ A solution of 2-gb (0.2 g, 1.15 mmol) in 10 ml CH_3OH was added dropwise to a solution of $H_3PMo_{12}O_{40}$ (2.1 g, 1.15 mmol) in CH_3CN (60 ml) and stirred (1 h). Filtrating, the solution was kept in a beaker. After a few days, the produced solid was recrystallizes in a mixture of CH_3OH—H_2O—CH_2Cl_2 (4:1:1). A dark red crystal was obtained with slow evaporation. All mentioned process was done at room temperature. Elemental analysis (%) calcd. for $C_{10.5}H_{30}Mo_{12}N_5O_{46.5}P$: C 5.86, H 1.40, N 3.25; found: C 5.75, H 1.36, N 3.21. ^{1}H NMR (500.13 MHz, [D_6]DMSO, 298 K, TMS): 3.16 (s, CH_3, 7.5H), 5.12 (b, NH, OH, H^+, 18.5H), 7.12–7.71 (m, C_6H_4, 4H). ^{13}C NMR (125.77 MHz, [D_6]DMSO, 298 K, TMS): 159.10, 150.28, 132.31, 123.03, 112.25, 48.72. IR (KBr, cm^{-1}): 3385, 1687, 1621, 1519, 1451, 1056, 955, 873, 790, 610, 588, 491.

Refinement

There is a high positive residual density of 1.67 e $Å^{-3}$ near the Mo8 center (distance 0.87%A) due to considerable absorption effects which could not be completely corrected. All solvent molecules were refind in isotropic approximation becouse of high disorder. The hydrogen atoms of NH_2, NH and OH groups, and also H atoms of water molecules were found in difference Fourier synthesis, the H(C) atom positions were calculated. All hydrogen atoms were refined in isotropic approximation in riding model with with the U_{iso}(H) parameters equal to 1.2 U_{eq}(Ci), for methyl groups equal to 1.5 U_{eq}(Ci), where U(Ci) are the equivalent thermal parameters of the carbon atoms to which corresponding H atoms are bonded.

Figures

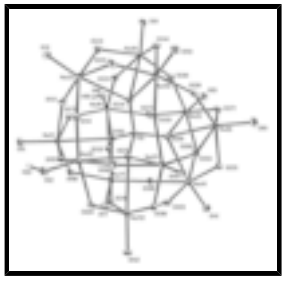

Fig. 1. The molecular structure of the $[H_2PMo_{12}O_{40}]^-$ anion with displacement ellipsoids drawn at the 50% probability level.

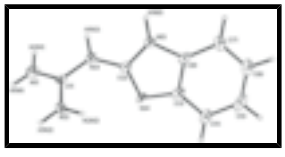

Fig. 2. The molecular structure of the $[C_8H_9N_5]^+$ cation with displacement ellipsoids drawn at the 50% probability level.

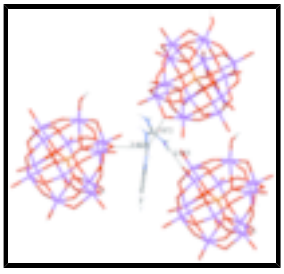

Fig. 3. Location of 2-gbH$^+$ cation between three heteropolyanions, solvated H_2O and CH_3OH molecules are omitted for clarity.

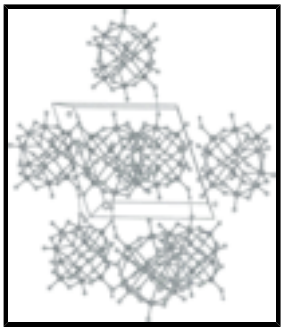

Fig. 4. Crystal packing of anions (along *b* crystal axis) in the structure of title compound.

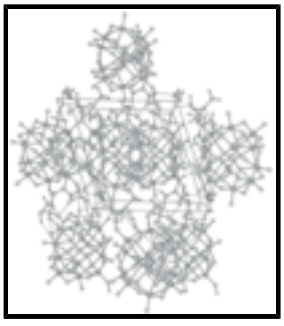

Fig. 5. Crystal packing (along *b* crystal axis) in the structure of title compound. Hydrogen bonds are shown with dashed lines.

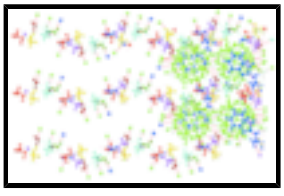

Fig. 6. A view of the infinite zigzag belts around the organic cations and inorganic anions with sequence $H_2O\cdots CH_3OH\cdots H_2O\cdots H_2O\cdots CH_3OH\cdots CH_3OH\cdots CH_3OH\cdots$ in the chains (some organic cations and inorganic anions are given in Figure for showing the position of them relative to solvated molecules).

1-(1*H*-1,3-benzimidazol-2-yl)guanidinium dihydrogendodecamolybdophosphate–methanol–water (1:2.5:4)

Crystal data

$(C_8H_{10}N_5)[H_2PMo_{12}O_{40}]\cdot 2.5CH_4O\cdot 4H_2O$	F_{000} = 2038
M_r = 2152.65	D_x = 2.734 Mg m^{-3}
Monoclinic, $P2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2yb	Cell parameters from 7125 reflections
a = 11.9025 (12) Å	θ = 2.3–30.0º
b = 18.2497 (19) Å	μ = 2.92 mm^{-1}
c = 12.7798 (13) Å	T = 120 (2) K
β = 109.639 (2)º	Plate, orange
V = 2614.5 (5) Å^3	0.40 × 0.30 × 0.15 mm

$Z = 2$

Data collection

Bruker SMART 1000 CCD area-detector diffractometer	9960 independent reflections
Radiation source: fine-focus sealed tube	9679 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.093$
$T = 120(2)$ K	$\theta_{max} = 26.0^{o}$
φ and ω scans	$\theta_{min} = 2.0^{o}$
Absorption correction: multi scan (SADABS; Sheldrick, 1998a)	$h = -14 \rightarrow 14$
$T_{min} = 0.360$, $T_{max} = 0.648$	$k = -22 \rightarrow 22$
22667 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Hydrogen site location: mixed
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.043$	$w = 1/[\sigma^2(F_o^2) + (0.01P)^2 + 25P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.095$	$(\Delta/\sigma)_{max} = 0.002$
$S = 1.05$	$\Delta\rho_{max} = 1.68$ e Å^{-3}
9960 reflections	$\Delta\rho_{min} = -1.28$ e Å^{-3}
663 parameters	Extinction correction: none
30 restraints	Absolute structure: Flack (1983), 4793 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.04 (5)
Secondary atom site location: difference Fourier map	

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}	Occ. (<1)
Mo1	0.43252 (7)	0.20089 (4)	0.85557 (6)	0.01435 (15)	
Mo2	0.29456 (7)	0.38543 (4)	0.79544 (6)	0.01441 (15)	
Mo3	0.21469 (7)	0.24071 (4)	0.57690 (6)	0.01526 (15)	

Mo4	0.79103 (7)	0.40358 (4)	0.74839 (6)	0.01442 (15)
Mo5	0.71946 (7)	0.27090 (4)	0.54842 (6)	0.01445 (15)
Mo6	0.58973 (7)	0.43942 (4)	0.48978 (6)	0.01366 (14)
Mo7	0.72301 (7)	0.25501 (4)	0.91725 (6)	0.01427 (15)
Mo8	0.59978 (7)	0.13609 (4)	0.70229 (6)	0.01449 (15)
Mo9	0.40501 (7)	0.20860 (4)	0.43064 (6)	0.01466 (15)
Mo10	0.27665 (7)	0.37756 (4)	0.42193 (6)	0.01454 (15)
Mo11	0.40734 (7)	0.50829 (4)	0.65420 (6)	0.01382 (15)
Mo12	0.58664 (7)	0.44000 (4)	0.90565 (6)	0.01383 (15)
P1	0.5035 (2)	0.32237 (12)	0.67082 (18)	0.0125 (4)
O1	0.3700 (6)	0.1488 (3)	0.9304 (5)	0.0212 (14)
O2	0.1919 (6)	0.3958 (4)	0.8580 (6)	0.0235 (14)
H2	0.1091	0.4047	0.8463	0.028*
O3	0.0785 (6)	0.2075 (4)	0.5587 (5)	0.0219 (13)
O4	0.9269 (6)	0.4366 (4)	0.8110 (5)	0.0204 (13)
O5	0.8004 (6)	0.2308 (3)	0.4782 (5)	0.0193 (13)
O6	0.6060 (6)	0.5045 (3)	0.4042 (5)	0.0195 (13)
O7	0.8325 (6)	0.2428 (4)	1.0398 (5)	0.0210 (13)
O8	0.6548 (6)	0.0528 (3)	0.6932 (5)	0.0191 (13)
H8	0.6864	0.0087	0.7330	0.023*
O9	0.3830 (6)	0.1458 (3)	0.3299 (5)	0.0196 (13)
O10	0.1877 (6)	0.4178 (3)	0.3061 (5)	0.0198 (13)
O11	0.3516 (6)	0.5925 (3)	0.6152 (5)	0.0177 (13)
O12	0.6546 (6)	0.4913 (3)	1.0182 (5)	0.0208 (14)
O13	0.3113 (6)	0.1953 (3)	0.7048 (5)	0.0171 (12)
O14	0.2217 (6)	0.3266 (3)	0.6772 (5)	0.0181 (13)
O15	0.3744 (6)	0.2915 (3)	0.8642 (5)	0.0174 (13)
O16	0.5853 (6)	0.2139 (3)	0.9549 (5)	0.0160 (12)
O17	0.5052 (6)	0.1198 (3)	0.7902 (5)	0.0196 (13)
O18	0.5455 (5)	0.2576 (3)	0.7507 (4)	0.0128 (11)
O19	0.2874 (6)	0.4727 (4)	0.7224 (5)	0.0181 (13)
O20	0.4358 (5)	0.4269 (3)	0.9164 (5)	0.0162 (12)
O21	0.4655 (6)	0.3861 (3)	0.7320 (5)	0.0172 (12)
O22	0.1704 (6)	0.3195 (3)	0.4620 (5)	0.0200 (13)
O23	0.2627 (6)	0.1859 (3)	0.4784 (5)	0.0185 (13)
O24	0.3967 (5)	0.2980 (3)	0.5699 (5)	0.0127 (11)
O25	0.7379 (6)	0.4606 (3)	0.6209 (5)	0.0201 (14)
O26	0.8308 (5)	0.3270 (3)	0.6541 (5)	0.0161 (12)
O27	0.6750 (6)	0.3628 (4)	0.4582 (5)	0.0187 (13)
O28	0.6055 (6)	0.3479 (3)	0.6309 (5)	0.0152 (12)
O29	0.4402 (6)	0.4037 (3)	0.4229 (5)	0.0159 (12)
O30	0.5173 (5)	0.4958 (3)	0.5852 (5)	0.0152 (12)
O31	0.6474 (6)	0.3495 (3)	0.9459 (5)	0.0162 (12)
O32	0.7266 (6)	0.1693 (3)	0.8436 (5)	0.0168 (12)
O33	0.4851 (6)	0.1510 (3)	0.5694 (5)	0.0184 (13)
O34	0.3147 (6)	0.2853 (3)	0.3528 (5)	0.0153 (12)
O35	0.3003 (5)	0.4467 (3)	0.5275 (5)	0.0171 (12)
O36	0.5083 (5)	0.5228 (3)	0.7980 (5)	0.0143 (12)
O37	0.7012 (6)	0.1992 (3)	0.6402 (5)	0.0170 (12)

O38	0.7906 (6)	0.3159 (3)	0.8407 (5)	0.0170 (13)	
O39	0.5529 (6)	0.2441 (3)	0.4510 (5)	0.0163 (12)	
O40	0.7004 (6)	0.4458 (3)	0.8223 (5)	0.0165 (12)	
N1	0.9071 (9)	0.0675 (6)	0.2019 (8)	0.037 (2)	
H1N1	0.9820	0.0576	0.2403	0.045*	
H2N1	0.8735	0.0479	0.1358	0.045*	
N2	0.8895 (8)	0.1424 (5)	0.3404 (7)	0.031 (2)	
H1N2	0.9642	0.1337	0.3812	0.037*	
H2N2	0.8454	0.1715	0.3654	0.037*	
N3	0.7277 (7)	0.1256 (4)	0.1769 (6)	0.0232 (17)	
H1N3	0.6929	0.0937	0.1218	0.028*	
N4	0.6957 (8)	0.2533 (4)	0.2111 (6)	0.0218 (17)	
N5	0.5432 (7)	0.1773 (4)	0.1600 (6)	0.0209 (16)	
H1N5	0.4994	0.1365	0.1365	0.025*	
C1	0.8436 (9)	0.1112 (5)	0.2414 (7)	0.0202 (19)	
C2	0.6601 (10)	0.1846 (5)	0.1869 (8)	0.024 (2)	
C3	0.5923 (10)	0.2948 (6)	0.1954 (8)	0.026 (2)	
C4	0.5792 (11)	0.3697 (6)	0.2064 (8)	0.030 (2)	
H4A	0.6456	0.4020	0.2292	0.035*	
C5	0.4617 (12)	0.3947 (7)	0.1817 (9)	0.039 (3)	
H5A	0.4483	0.4453	0.1904	0.047*	
C6	0.3656 (11)	0.3484 (7)	0.1452 (8)	0.035 (3)	
H6A	0.2874	0.3679	0.1273	0.042*	
C7	0.3799 (10)	0.2729 (6)	0.1339 (8)	0.030 (2)	
H7A	0.3137	0.2405	0.1085	0.036*	
C8	0.4950 (11)	0.2487 (6)	0.1618 (7)	0.029 (2)	
C1S	1.0586 (16)	0.2459 (9)	0.8299 (15)	0.020 (4)*	0.50
H1SA	1.1420	0.2358	0.8472	0.030*	0.50
H1SB	1.0222	0.2526	0.7512	0.030*	0.50
H1SC	1.0490	0.2896	0.8678	0.030*	0.50
O1S	1.0024 (16)	0.1884 (9)	0.8658 (15)	0.047 (4)*	0.50
H1OS	0.9192	0.1978	0.8447	0.056*	0.50
C2S	−0.0769 (16)	0.0770 (12)	0.6403 (14)	0.025 (4)*	0.50
H2SA	−0.1509	0.0934	0.6470	0.038*	0.50
H2SB	−0.0613	0.1038	0.5821	0.038*	0.50
H2SC	−0.0822	0.0256	0.6230	0.038*	0.50
O2S	0.0166 (16)	0.0863 (12)	0.7421 (14)	0.060 (5)*	0.50
H2OS	0.0795	0.0575	0.7917	0.072*	0.50
C3S	0.1712 (15)	0.0995 (9)	0.0969 (15)	0.019 (4)*	0.50
H3SA	0.1753	0.0723	0.0340	0.029*	0.50
H3SB	0.2494	0.1169	0.1395	0.029*	0.50
H3SC	0.1420	0.0683	0.1425	0.029*	0.50
O3S	0.0958 (16)	0.1602 (9)	0.0616 (16)	0.051 (5)*	0.50
H3OS	0.0227	0.1411	0.0106	0.061*	0.50
C4S	0.984 (2)	0.4172 (16)	0.5329 (17)	0.048 (6)*	0.50
H4SA	1.0535	0.4337	0.5179	0.072*	0.50
H4SB	0.9639	0.4520	0.5803	0.072*	0.50
H4SC	0.9996	0.3704	0.5691	0.072*	0.50
O4S	0.8901 (16)	0.4078 (10)	0.4337 (14)	0.047 (4)*	0.50

H4OS	0.8047	0.4067	0.4131	0.057*	0.50
C5S	0.915 (3)	0.5326 (15)	0.551 (2)	0.057 (7)*	0.50
H5SA	0.8527	0.4976	0.5188	0.086*	0.50
H5SB	0.9879	0.5072	0.5894	0.086*	0.50
H5SC	0.9257	0.5629	0.4941	0.086*	0.50
O5S	0.8835 (14)	0.5782 (9)	0.6248 (12)	0.034 (3)*	0.50
H5OS	0.8259	0.5950	0.6568	0.041*	0.50
O1W	0.6451 (6)	0.0420 (4)	−0.0092 (5)	0.0226 (14)*	
H1W1	0.5992	−0.0050	−0.0125	0.027*	
H2W1	0.7186	0.0299	−0.0284	0.027*	
O2W	0.9124 (9)	0.3210 (5)	0.2657 (8)	0.025 (2)*	0.70
H2W2	0.8450	0.2856	0.2586	0.030*	0.70
H1W2	0.8814	0.3652	0.2169	0.030*	0.70
O2W'	0.903 (3)	0.3913 (17)	0.181 (2)	0.045 (7)*	0.30
H1W'	0.9349	0.3825	0.1186	0.054*	0.30
H2W'	0.8386	0.4299	0.1696	0.054*	0.30
O3W	0.0782 (14)	0.2291 (9)	0.2349 (13)	0.035 (4)*	0.50
H1W3	0.0989	0.2672	0.1870	0.042*	0.50
H2W3	0.0992	0.1797	0.2111	0.042*	0.50
O4W	0.2188 (17)	0.0358 (10)	0.7131 (15)	0.045 (4)*	0.50
H1W4	0.2638	0.0604	0.6685	0.054*	0.50
H2W4	0.1340	0.0496	0.7044	0.054*	0.50
O5W	0.1067 (17)	0.5645 (11)	0.0276 (15)	0.062 (4)*	0.60
H3W'	0.0623	0.5277	0.0581	0.074*	0.60
H4W'	0.1503	0.6060	0.0767	0.074*	0.60
O5W'	0.128 (3)	0.5022 (17)	0.058 (2)	0.066 (7)*	0.40
H5W'	0.0630	0.4744	0.0765	0.079*	0.40
H6W'	0.1389	0.5414	0.1171	0.079*	0.40

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Mo1	0.0219 (4)	0.0110 (3)	0.0092 (3)	−0.0009 (3)	0.0040 (3)	0.0010 (3)
Mo2	0.0199 (4)	0.0123 (3)	0.0111 (3)	0.0000 (3)	0.0054 (3)	−0.0001 (3)
Mo3	0.0195 (4)	0.0133 (3)	0.0109 (3)	−0.0019 (3)	0.0023 (3)	−0.0005 (3)
Mo4	0.0183 (4)	0.0125 (3)	0.0111 (3)	−0.0016 (3)	0.0032 (3)	−0.0009 (3)
Mo5	0.0212 (4)	0.0117 (3)	0.0105 (3)	0.0022 (3)	0.0054 (3)	0.0002 (3)
Mo6	0.0211 (4)	0.0098 (3)	0.0102 (3)	0.0008 (3)	0.0055 (3)	0.0015 (3)
Mo7	0.0203 (4)	0.0118 (3)	0.0086 (3)	0.0001 (3)	0.0021 (3)	0.0003 (3)
Mo8	0.0230 (4)	0.0091 (3)	0.0095 (3)	0.0007 (3)	0.0031 (3)	−0.0002 (3)
Mo9	0.0226 (4)	0.0112 (3)	0.0080 (3)	0.0006 (3)	0.0023 (3)	−0.0012 (3)
Mo10	0.0203 (4)	0.0120 (3)	0.0086 (3)	0.0017 (3)	0.0011 (3)	0.0004 (3)
Mo11	0.0204 (4)	0.0093 (3)	0.0112 (3)	0.0007 (3)	0.0046 (3)	−0.0001 (3)
Mo12	0.0214 (4)	0.0103 (3)	0.0089 (3)	−0.0007 (3)	0.0039 (3)	−0.0024 (3)
P1	0.0203 (10)	0.0080 (9)	0.0081 (8)	0.0004 (8)	0.0036 (8)	−0.0010 (7)
O1	0.030 (4)	0.017 (3)	0.019 (3)	−0.007 (3)	0.012 (3)	0.002 (3)
O2	0.028 (3)	0.020 (3)	0.025 (3)	0.000 (3)	0.012 (3)	0.001 (3)
O3	0.025 (3)	0.020 (3)	0.020 (3)	−0.005 (3)	0.006 (3)	−0.001 (3)

O4	0.025 (3)	0.015 (3)	0.020 (3)	0.000 (3)	0.005 (3)	0.002 (3)
O5	0.025 (3)	0.019 (3)	0.017 (3)	0.005 (3)	0.010 (3)	−0.004 (2)
O6	0.032 (4)	0.012 (3)	0.015 (3)	0.005 (3)	0.010 (3)	0.005 (2)
O7	0.029 (3)	0.017 (3)	0.011 (3)	0.000 (3)	0.000 (3)	−0.006 (2)
O8	0.028 (3)	0.011 (3)	0.018 (3)	0.006 (3)	0.007 (3)	0.004 (2)
O9	0.029 (3)	0.015 (3)	0.013 (3)	0.001 (3)	0.005 (3)	0.001 (2)
O10	0.028 (3)	0.016 (3)	0.009 (3)	0.003 (3)	−0.001 (3)	0.004 (2)
O11	0.027 (3)	0.010 (3)	0.015 (3)	0.001 (2)	0.007 (3)	0.004 (2)
O12	0.036 (4)	0.011 (3)	0.011 (3)	−0.006 (3)	0.003 (3)	−0.005 (2)
O13	0.023 (3)	0.012 (3)	0.013 (3)	−0.003 (3)	0.001 (2)	0.000 (2)
O14	0.021 (3)	0.017 (3)	0.013 (3)	−0.002 (3)	0.002 (3)	0.005 (2)
O15	0.026 (3)	0.013 (3)	0.012 (3)	0.005 (3)	0.005 (3)	0.000 (2)
O16	0.030 (3)	0.012 (3)	0.006 (3)	−0.003 (3)	0.006 (2)	0.002 (2)
O17	0.032 (4)	0.010 (3)	0.015 (3)	−0.002 (3)	0.007 (3)	0.003 (2)
O18	0.014 (3)	0.014 (3)	0.008 (2)	−0.001 (2)	0.000 (2)	−0.002 (2)
O19	0.022 (3)	0.020 (3)	0.013 (3)	0.002 (3)	0.008 (3)	0.001 (2)
O20	0.022 (3)	0.019 (3)	0.007 (3)	0.000 (3)	0.003 (2)	0.001 (2)
O21	0.029 (3)	0.008 (3)	0.014 (3)	−0.001 (2)	0.007 (3)	−0.001 (2)
O22	0.029 (3)	0.016 (3)	0.017 (3)	0.000 (3)	0.011 (3)	0.001 (2)
O23	0.028 (3)	0.013 (3)	0.015 (3)	0.000 (3)	0.007 (3)	0.000 (2)
O24	0.017 (3)	0.010 (3)	0.008 (3)	0.002 (2)	−0.001 (2)	0.000 (2)
O25	0.034 (4)	0.012 (3)	0.021 (3)	0.000 (3)	0.018 (3)	0.003 (2)
O26	0.016 (3)	0.016 (3)	0.017 (3)	0.001 (2)	0.005 (3)	−0.001 (2)
O27	0.028 (3)	0.019 (3)	0.008 (3)	0.002 (3)	0.005 (2)	−0.003 (2)
O28	0.024 (3)	0.008 (3)	0.009 (3)	0.001 (2)	−0.001 (2)	−0.003 (2)
O29	0.028 (3)	0.011 (3)	0.011 (3)	0.001 (3)	0.009 (3)	0.002 (2)
O30	0.021 (3)	0.017 (3)	0.008 (3)	0.002 (2)	0.004 (2)	0.002 (2)
O31	0.023 (3)	0.010 (3)	0.013 (3)	0.002 (2)	0.001 (3)	0.003 (2)
O32	0.021 (3)	0.014 (3)	0.014 (3)	0.010 (2)	0.004 (3)	0.005 (2)
O33	0.024 (3)	0.014 (3)	0.017 (3)	−0.001 (3)	0.007 (3)	−0.003 (2)
O34	0.022 (3)	0.012 (3)	0.008 (3)	−0.001 (2)	0.000 (2)	−0.002 (2)
O35	0.020 (3)	0.016 (3)	0.015 (3)	0.003 (3)	0.006 (3)	0.004 (2)
O36	0.018 (3)	0.010 (3)	0.015 (3)	−0.001 (2)	0.006 (2)	0.000 (2)
O37	0.022 (3)	0.017 (3)	0.009 (3)	0.004 (3)	0.002 (2)	0.001 (2)
O38	0.022 (3)	0.017 (3)	0.013 (3)	0.005 (3)	0.006 (3)	0.006 (2)
O39	0.020 (3)	0.015 (3)	0.009 (3)	0.001 (2)	−0.002 (2)	−0.002 (2)
O40	0.023 (3)	0.015 (3)	0.011 (3)	0.003 (3)	0.005 (2)	0.000 (2)
N1	0.031 (5)	0.047 (6)	0.037 (5)	−0.006 (4)	0.015 (4)	−0.021 (5)
N2	0.025 (4)	0.039 (5)	0.025 (4)	0.008 (4)	0.004 (4)	−0.014 (4)
N3	0.031 (4)	0.023 (4)	0.013 (4)	0.008 (4)	0.003 (3)	0.001 (3)
N4	0.040 (5)	0.008 (3)	0.015 (4)	0.001 (3)	0.006 (3)	−0.002 (3)
N5	0.021 (4)	0.023 (4)	0.011 (4)	−0.007 (3)	−0.003 (3)	−0.005 (3)
C1	0.028 (4)	0.024 (4)	0.010 (4)	−0.009 (3)	0.008 (3)	−0.008 (3)
C2	0.044 (6)	0.017 (5)	0.018 (4)	0.000 (4)	0.020 (4)	0.002 (4)
C3	0.049 (6)	0.021 (5)	0.012 (4)	−0.006 (4)	0.015 (4)	−0.001 (4)
C4	0.049 (6)	0.026 (5)	0.014 (4)	0.004 (5)	0.011 (4)	0.005 (4)
C5	0.064 (6)	0.034 (5)	0.020 (4)	0.014 (5)	0.015 (4)	0.007 (4)
C6	0.040 (5)	0.047 (5)	0.017 (4)	0.012 (4)	0.009 (4)	0.004 (4)
C7	0.037 (6)	0.037 (6)	0.014 (4)	0.011 (5)	0.006 (4)	0.006 (4)

C8	0.052 (7)	0.026 (5)	0.011 (4)	−0.003 (5)	0.014 (4)	0.003 (4)

Geometric parameters (Å, °)

Mo1—O1	1.689 (6)	P1—O18	1.531 (6)
Mo1—O15	1.811 (6)	P1—O28	1.539 (7)
Mo1—O16	1.850 (6)	P1—O24	1.541 (6)
Mo1—O13	1.984 (6)	P1—O21	1.550 (6)
Mo1—O17	2.030 (6)	O2—H2	0.9600
Mo1—O18	2.427 (6)	O8—H8	0.9601
Mo2—O2	1.680 (6)	N1—C1	1.311 (13)
Mo2—O14	1.818 (6)	N1—H1N1	0.8803
Mo2—O19	1.833 (6)	N1—H2N1	0.8798
Mo2—O20	2.010 (6)	N2—C1	1.326 (12)
Mo2—O15	2.012 (6)	N2—H1N2	0.8799
Mo2—O21	2.431 (6)	N2—H2N2	0.8799
Mo3—O3	1.672 (7)	N3—C1	1.374 (13)
Mo3—O23	1.843 (6)	N3—C2	1.375 (12)
Mo3—O13	1.848 (6)	N3—H1N3	0.8999
Mo3—O22	1.995 (6)	N4—C2	1.327 (12)
Mo3—O14	2.009 (6)	N4—C3	1.401 (14)
Mo3—O24	2.434 (6)	N5—C2	1.324 (14)
Mo4—O4	1.658 (7)	N5—C8	1.426 (14)
Mo4—O40	1.826 (6)	N5—H1N5	0.9011
Mo4—O25	1.856 (6)	C3—C8	1.378 (15)
Mo4—O38	1.989 (6)	C3—C4	1.388 (15)
Mo4—O26	2.004 (6)	C4—C5	1.402 (17)
Mo4—O28	2.436 (6)	C4—H4A	0.9500
Mo5—O5	1.688 (6)	C5—C6	1.372 (18)
Mo5—O37	1.818 (6)	C5—H5A	0.9500
Mo5—O26	1.851 (6)	C6—C7	1.401 (17)
Mo5—O27	2.003 (6)	C6—H6A	0.9500
Mo5—O39	2.015 (6)	C7—C8	1.368 (16)
Mo5—O28	2.426 (6)	C7—H7A	0.9500
Mo6—O6	1.670 (6)	C1S—O1S	1.402 (10)
Mo6—O29	1.816 (6)	C1S—H1SA	0.9598
Mo6—O27	1.850 (6)	C1S—H1SB	0.9603
Mo6—O30	1.998 (6)	C1S—H1SC	0.9601
Mo6—O25	2.021 (7)	O1S—H1OS	0.9499
Mo6—O28	2.419 (6)	C2S—O2S	1.410 (10)
Mo7—O7	1.682 (6)	C2S—H2SA	0.9605
Mo7—O32	1.834 (6)	C2S—H2SB	0.9601
Mo7—O38	1.835 (6)	C2S—H2SC	0.9596
Mo7—O16	2.003 (6)	O2S—H2OS	0.9598
Mo7—O31	2.035 (6)	C3S—O3S	1.401 (10)
Mo7—O18	2.444 (6)	C3S—H3SA	0.9601
Mo8—O8	1.674 (6)	C3S—H3SB	0.9602
Mo8—O33	1.806 (6)	C3S—H3SC	0.9596
Mo8—O17	1.862 (6)	O3S—H3OS	0.9598

Mo8—O37	2.015 (6)	C4S—O4S	1.390 (10)
Mo8—O32	2.018 (6)	C4S—H4SA	0.9599
Mo8—O18	2.447 (6)	C4S—H4SB	0.9601
Mo9—O9	1.677 (6)	C4S—H4SC	0.9600
Mo9—O39	1.810 (6)	O4S—H4OS	0.9599
Mo9—O34	1.840 (6)	C5S—O5S	1.395 (10)
Mo9—O33	2.006 (6)	C5S—H5SA	0.9600
Mo9—O23	2.026 (6)	C5S—H5SB	0.9601
Mo9—O24	2.440 (6)	C5S—H5SC	0.9600
Mo10—O10	1.673 (6)	O5S—H5OS	0.9599
Mo10—O35	1.799 (6)	O1W—H1W1	1.0101
Mo10—O22	1.849 (6)	O1W—H2W1	1.0095
Mo10—O29	2.001 (6)	O2W—H2W2	1.0101
Mo10—O34	2.023 (6)	O2W—H1W2	1.0101
Mo10—O24	2.431 (6)	O2W'—H1W2	0.7595
Mo11—O11	1.681 (6)	O2W'—H1W'	1.0098
Mo11—O30	1.822 (6)	O2W'—H2W'	1.0102
Mo11—O36	1.845 (6)	O3W—H1W3	1.0099
Mo11—O19	2.014 (6)	O3W—H2W3	1.0099
Mo11—O35	2.030 (6)	O4W—H1W4	1.0099
Mo11—O21	2.446 (6)	O4W—H2W4	1.0100
Mo12—O12	1.679 (6)	O5W—H3W'	1.0097
Mo12—O31	1.806 (6)	O5W—H4W'	1.0102
Mo12—O20	1.862 (6)	O5W—H6W'	1.1570
Mo12—O40	1.987 (6)	O5W'—H3W'	0.9128
Mo12—O36	2.046 (6)	O5W'—H5W'	1.0200
Mo12—O21	2.413 (6)	O5W'—H6W'	1.0201
O1—Mo1—O15	103.3 (3)	O36—Mo11—O21	74.1 (2)
O1—Mo1—O16	101.7 (3)	O19—Mo11—O21	71.0 (2)
O15—Mo1—O16	98.5 (3)	O35—Mo11—O21	80.5 (2)
O1—Mo1—O13	101.9 (3)	O12—Mo12—O31	103.6 (3)
O15—Mo1—O13	86.4 (3)	O12—Mo12—O20	102.0 (3)
O16—Mo1—O13	154.1 (3)	O31—Mo12—O20	99.5 (3)
O1—Mo1—O17	98.8 (3)	O12—Mo12—O40	102.1 (3)
O15—Mo1—O17	156.2 (3)	O31—Mo12—O40	85.5 (3)
O16—Mo1—O17	85.4 (3)	O20—Mo12—O40	153.4 (3)
O13—Mo1—O17	80.5 (3)	O12—Mo12—O36	98.3 (3)
O1—Mo1—O18	170.0 (3)	O31—Mo12—O36	156.2 (2)
O15—Mo1—O18	86.4 (2)	O20—Mo12—O36	84.9 (2)
O16—Mo1—O18	74.1 (2)	O40—Mo12—O36	80.7 (2)
O13—Mo1—O18	80.9 (2)	O12—Mo12—O21	169.3 (3)
O17—Mo1—O18	72.1 (2)	O31—Mo12—O21	87.0 (2)
O2—Mo2—O14	104.0 (3)	O20—Mo12—O21	73.9 (2)
O2—Mo2—O19	103.1 (3)	O40—Mo12—O21	80.4 (2)
O14—Mo2—O19	99.3 (3)	O36—Mo12—O21	71.7 (2)
O2—Mo2—O20	98.4 (3)	O18—P1—O28	109.7 (3)
O14—Mo2—O20	154.6 (3)	O18—P1—O24	109.1 (3)
O19—Mo2—O20	87.0 (3)	O28—P1—O24	109.3 (3)
O2—Mo2—O15	101.6 (3)	O18—P1—O21	109.1 (3)

O14—Mo2—O15	83.3 (3)	O28—P1—O21	109.6 (3)
O19—Mo2—O15	153.7 (3)	O24—P1—O21	109.9 (3)
O20—Mo2—O15	80.5 (3)	Mo2—O2—H2	144.9
O2—Mo2—O21	169.2 (3)	Mo8—O8—H8	144.9
O14—Mo2—O21	86.8 (2)	Mo3—O13—Mo1	150.4 (3)
O19—Mo2—O21	74.1 (2)	Mo2—O14—Mo3	153.8 (4)
O20—Mo2—O21	71.2 (2)	Mo1—O15—Mo2	152.3 (3)
O15—Mo2—O21	79.9 (2)	Mo1—O16—Mo7	125.3 (3)
O3—Mo3—O23	102.6 (3)	Mo8—O17—Mo1	124.0 (3)
O3—Mo3—O13	104.3 (3)	P1—O18—Mo1	125.5 (3)
O23—Mo3—O13	96.7 (3)	P1—O18—Mo7	126.1 (3)
O3—Mo3—O22	98.9 (3)	Mo1—O18—Mo7	89.30 (18)
O23—Mo3—O22	87.4 (3)	P1—O18—Mo8	125.8 (3)
O13—Mo3—O22	154.9 (3)	Mo1—O18—Mo8	89.7 (2)
O3—Mo3—O14	101.7 (3)	Mo7—O18—Mo8	88.73 (19)
O23—Mo3—O14	154.6 (3)	Mo2—O19—Mo11	125.6 (3)
O13—Mo3—O14	84.6 (3)	Mo12—O20—Mo2	124.7 (3)
O22—Mo3—O14	81.4 (2)	P1—O21—Mo12	125.8 (4)
O3—Mo3—O24	169.7 (3)	P1—O21—Mo2	125.7 (3)
O23—Mo3—O24	73.9 (2)	Mo12—O21—Mo2	90.19 (19)
O13—Mo3—O24	85.9 (2)	P1—O21—Mo11	124.7 (3)
O22—Mo3—O24	71.4 (2)	Mo12—O21—Mo11	90.1 (2)
O14—Mo3—O24	80.9 (2)	Mo2—O21—Mo11	89.2 (2)
O4—Mo4—O40	104.3 (3)	Mo10—O22—Mo3	125.5 (4)
O4—Mo4—O25	102.1 (3)	Mo3—O23—Mo9	125.3 (3)
O40—Mo4—O25	97.5 (3)	P1—O24—Mo10	125.6 (3)
O4—Mo4—O38	101.7 (3)	P1—O24—Mo3	125.9 (3)
O40—Mo4—O38	85.0 (3)	Mo10—O24—Mo3	89.3 (2)
O25—Mo4—O38	154.7 (3)	P1—O24—Mo9	125.4 (3)
O4—Mo4—O26	98.9 (3)	Mo10—O24—Mo9	89.39 (19)
O40—Mo4—O26	154.9 (3)	Mo3—O24—Mo9	89.7 (2)
O25—Mo4—O26	86.7 (3)	Mo4—O25—Mo6	124.4 (3)
O38—Mo4—O26	81.0 (2)	Mo5—O26—Mo4	124.7 (3)
O4—Mo4—O28	169.8 (3)	Mo6—O27—Mo5	124.5 (3)
O40—Mo4—O28	85.7 (2)	P1—O28—Mo6	125.7 (3)
O25—Mo4—O28	73.9 (3)	P1—O28—Mo5	126.0 (3)
O38—Mo4—O28	81.2 (2)	Mo6—O28—Mo5	89.5 (2)
O26—Mo4—O28	71.7 (2)	P1—O28—Mo4	125.1 (3)
O5—Mo5—O37	104.1 (3)	Mo6—O28—Mo4	89.9 (2)
O5—Mo5—O26	103.3 (3)	Mo5—O28—Mo4	89.2 (2)
O37—Mo5—O26	98.0 (3)	Mo6—O29—Mo10	152.3 (3)
O5—Mo5—O27	98.3 (3)	Mo11—O30—Mo6	152.6 (4)
O37—Mo5—O27	155.2 (3)	Mo12—O31—Mo7	151.9 (3)
O26—Mo5—O27	86.7 (3)	Mo7—O32—Mo8	125.2 (3)
O5—Mo5—O39	100.7 (3)	Mo8—O33—Mo9	153.5 (4)
O37—Mo5—O39	85.3 (3)	Mo9—O34—Mo10	124.9 (3)
O26—Mo5—O39	154.1 (3)	Mo10—O35—Mo11	152.2 (4)
O27—Mo5—O39	80.4 (3)	Mo11—O36—Mo12	124.1 (3)
O5—Mo5—O28	169.8 (3)	Mo5—O37—Mo8	152.0 (4)

O37—Mo5—O28	86.1 (2)	Mo7—O38—Mo4	153.2 (4)
O26—Mo5—O28	74.4 (2)	Mo9—O39—Mo5	152.0 (3)
O27—Mo5—O28	71.7 (2)	Mo4—O40—Mo12	151.9 (4)
O39—Mo5—O28	80.3 (2)	C1—N1—H1N1	121.2
O6—Mo6—O29	104.9 (3)	C1—N1—H2N1	118.8
O6—Mo6—O27	101.7 (3)	H1N1—N1—H2N1	120.0
O29—Mo6—O27	98.6 (3)	C1—N2—H1N2	119.9
O6—Mo6—O30	101.7 (3)	C1—N2—H2N2	120.1
O29—Mo6—O30	85.2 (3)	H1N2—N2—H2N2	120.0
O27—Mo6—O30	154.5 (3)	C1—N3—C2	126.5 (9)
O6—Mo6—O25	98.4 (3)	C1—N3—H1N3	116.8
O29—Mo6—O25	154.6 (2)	C2—N3—H1N3	116.7
O27—Mo6—O25	86.3 (3)	C2—N4—C3	106.3 (9)
O30—Mo6—O25	80.3 (2)	C2—N5—C8	107.3 (8)
O6—Mo6—O28	169.4 (3)	C2—N5—H1N5	127.5
O29—Mo6—O28	85.5 (2)	C8—N5—H1N5	124.8
O27—Mo6—O28	74.3 (2)	N1—C1—N2	121.5 (9)
O30—Mo6—O28	80.9 (2)	N1—C1—N3	118.5 (8)
O25—Mo6—O28	71.7 (2)	N2—C1—N3	120.0 (8)
O7—Mo7—O32	102.8 (3)	N5—C2—N4	112.4 (9)
O7—Mo7—O38	103.6 (3)	N5—C2—N3	119.7 (9)
O32—Mo7—O38	98.8 (3)	N4—C2—N3	127.6 (10)
O7—Mo7—O16	99.6 (3)	C8—C3—C4	121.4 (11)
O32—Mo7—O16	88.0 (3)	C8—C3—N4	108.7 (9)
O38—Mo7—O16	153.6 (3)	C4—C3—N4	129.9 (10)
O7—Mo7—O31	101.3 (3)	C3—C4—C5	115.8 (11)
O32—Mo7—O31	154.6 (3)	C3—C4—H4A	122.1
O38—Mo7—O31	83.2 (3)	C5—C4—H4A	122.1
O16—Mo7—O31	80.0 (2)	C6—C5—C4	122.1 (11)
O7—Mo7—O18	170.4 (3)	C6—C5—H5A	119.0
O32—Mo7—O18	74.5 (2)	C4—C5—H5A	119.0
O38—Mo7—O18	85.9 (2)	C5—C6—C7	121.6 (11)
O16—Mo7—O18	71.3 (2)	C5—C6—H6A	119.2
O31—Mo7—O18	80.5 (2)	C7—C6—H6A	119.2
O8—Mo8—O33	105.1 (3)	C8—C7—C6	115.8 (11)
O8—Mo8—O17	103.1 (3)	C8—C7—H7A	122.1
O33—Mo8—O17	99.9 (3)	C6—C7—H7A	122.1
O8—Mo8—O37	101.0 (3)	C7—C8—C3	123.2 (11)
O33—Mo8—O37	84.7 (3)	C7—C8—N5	131.5 (10)
O17—Mo8—O37	153.2 (3)	C3—C8—N5	105.2 (9)
O8—Mo8—O32	98.2 (3)	O1S—C1S—H1SA	110.6
O33—Mo8—O32	153.8 (3)	O1S—C1S—H1SB	110.0
O17—Mo8—O32	86.0 (3)	H1SA—C1S—H1SB	109.5
O37—Mo8—O32	79.3 (2)	O1S—C1S—H1SC	107.8
O8—Mo8—O18	169.4 (3)	H1SA—C1S—H1SC	109.5
O33—Mo8—O18	85.4 (2)	H1SB—C1S—H1SC	109.5
O17—Mo8—O18	74.2 (2)	C1S—O1S—H1OS	109.7
O37—Mo8—O18	80.0 (2)	O2S—C2S—H2SA	110.1
O32—Mo8—O18	71.6 (2)	O2S—C2S—H2SB	110.8

O9—Mo9—O39	104.4 (3)	H2SA—C2S—H2SB	109.4
O9—Mo9—O34	101.1 (3)	O2S—C2S—H2SC	107.6
O39—Mo9—O34	99.7 (3)	H2SA—C2S—H2SC	109.5
O9—Mo9—O33	103.1 (3)	H2SB—C2S—H2SC	109.5
O39—Mo9—O33	84.8 (3)	C2S—O2S—H2OS	137.9
O34—Mo9—O33	153.4 (2)	O3S—C3S—H3SA	110.3
O9—Mo9—O23	99.3 (3)	O3S—C3S—H3SB	108.3
O39—Mo9—O23	154.2 (3)	H3SA—C3S—H3SB	109.5
O34—Mo9—O23	85.6 (3)	O3S—C3S—H3SC	109.9
O33—Mo9—O23	79.8 (3)	H3SA—C3S—H3SC	109.5
O9—Mo9—O24	169.2 (3)	H3SB—C3S—H3SC	109.4
O39—Mo9—O24	86.1 (2)	C3S—O3S—H3OS	105.6
O34—Mo9—O24	74.1 (2)	O4S—C4S—H4SA	109.9
O33—Mo9—O24	80.2 (2)	O4S—C4S—H4SB	111.4
O23—Mo9—O24	71.0 (2)	H4SA—C4S—H4SB	109.5
O10—Mo10—O35	104.4 (3)	O4S—C4S—H4SC	107.2
O10—Mo10—O22	102.1 (3)	H4SA—C4S—H4SC	109.5
O35—Mo10—O22	98.2 (3)	H4SB—C4S—H4SC	109.5
O10—Mo10—O29	103.0 (3)	C4S—O4S—H4OS	134.8
O35—Mo10—O29	85.5 (3)	O5S—C5S—H4SB	124.0
O22—Mo10—O29	152.9 (3)	O5S—C5S—H5SA	110.3
O10—Mo10—O34	98.4 (3)	H4SB—C5S—H5SA	69.7
O35—Mo10—O34	155.5 (3)	O5S—C5S—H5SB	110.4
O22—Mo10—O34	85.3 (3)	H5SA—C5S—H5SB	109.5
O29—Mo10—O34	80.9 (2)	O5S—C5S—H5SC	107.7
O10—Mo10—O24	169.2 (3)	H4SB—C5S—H5SC	125.5
O35—Mo10—O24	86.2 (2)	H5SA—C5S—H5SC	109.5
O22—Mo10—O24	73.7 (3)	H5SB—C5S—H5SC	109.5
O29—Mo10—O24	79.7 (2)	C5S—O5S—H5OS	150.4
O34—Mo10—O24	71.5 (2)	H1W1—O1W—H2W1	107.8
O11—Mo11—O30	104.3 (3)	H2W2—O2W—H1W2	109.9
O11—Mo11—O36	102.9 (3)	H1W2—O2W'—H1W'	131.8
O30—Mo11—O36	99.6 (3)	H1W2—O2W'—H2W'	97.0
O11—Mo11—O19	99.0 (3)	H1W'—O2W'—H2W'	117.7
O30—Mo11—O19	153.9 (3)	H1W3—O3W—H2W3	107.2
O36—Mo11—O19	86.2 (3)	H1W4—O4W—H2W4	121.8
O11—Mo11—O35	101.0 (3)	H3W'—O5W—H4W'	119.0
O30—Mo11—O35	84.5 (3)	H3W'—O5W—H6W'	54.4
O36—Mo11—O35	153.9 (3)	H4W'—O5W—H6W'	74.3
O19—Mo11—O35	79.7 (2)	H3W'—O5W'—H5W'	62.1
O11—Mo11—O21	169.6 (3)	H3W'—O5W'—H6W'	62.0
O30—Mo11—O21	86.0 (2)	H5W'—O5W'—H6W'	95.1
O3—Mo3—O13—Mo1	−127.8 (7)	O23—Mo9—O24—P1	133.8 (4)
O23—Mo3—O13—Mo1	127.4 (7)	O9—Mo9—O24—Mo10	−65.4 (14)
O22—Mo3—O13—Mo1	29.1 (12)	O39—Mo9—O24—Mo10	100.8 (2)
O14—Mo3—O13—Mo1	−27.1 (7)	O34—Mo9—O24—Mo10	−0.5 (2)
O24—Mo3—O13—Mo1	54.1 (7)	O33—Mo9—O24—Mo10	−173.8 (2)
O1—Mo1—O13—Mo3	130.2 (7)	O23—Mo9—O24—Mo10	−91.2 (2)
O15—Mo1—O13—Mo3	27.3 (7)	O9—Mo9—O24—Mo3	23.9 (14)

O16—Mo1—O13—Mo3	−74.9 (10)	O39—Mo9—O24—Mo3	−169.9 (2)
O17—Mo1—O13—Mo3	−132.8 (7)	O34—Mo9—O24—Mo3	88.8 (2)
O18—Mo1—O13—Mo3	−59.6 (7)	O33—Mo9—O24—Mo3	−84.5 (2)
O2—Mo2—O14—Mo3	−133.1 (8)	O23—Mo9—O24—Mo3	−2.0 (2)
O19—Mo2—O14—Mo3	120.7 (8)	O4—Mo4—O25—Mo6	168.2 (4)
O20—Mo2—O14—Mo3	17.9 (12)	O40—Mo4—O25—Mo6	−85.3 (4)
O15—Mo2—O14—Mo3	−32.8 (8)	O38—Mo4—O25—Mo6	8.9 (8)
O21—Mo2—O14—Mo3	47.4 (8)	O26—Mo4—O25—Mo6	69.8 (4)
O3—Mo3—O14—Mo2	137.1 (8)	O28—Mo4—O25—Mo6	−2.1 (3)
O23—Mo3—O14—Mo2	−60.7 (11)	O6—Mo6—O25—Mo4	−173.8 (4)
O13—Mo3—O14—Mo2	33.6 (8)	O29—Mo6—O25—Mo4	29.7 (8)
O22—Mo3—O14—Mo2	−125.5 (8)	O27—Mo6—O25—Mo4	−72.6 (4)
O24—Mo3—O14—Mo2	−53.1 (8)	O30—Mo6—O25—Mo4	85.7 (4)
O1—Mo1—O15—Mo2	−129.9 (8)	O28—Mo6—O25—Mo4	2.1 (3)
O16—Mo1—O15—Mo2	125.9 (8)	O5—Mo5—O26—Mo4	168.2 (4)
O13—Mo1—O15—Mo2	−28.5 (8)	O37—Mo5—O26—Mo4	−85.2 (4)
O17—Mo1—O15—Mo2	27.9 (13)	O27—Mo5—O26—Mo4	70.4 (4)
O18—Mo1—O15—Mo2	52.7 (8)	O39—Mo5—O26—Mo4	10.4 (8)
O2—Mo2—O15—Mo1	132.6 (8)	O28—Mo5—O26—Mo4	−1.6 (3)
O14—Mo2—O15—Mo1	29.6 (8)	O4—Mo4—O26—Mo5	−174.2 (4)
O19—Mo2—O15—Mo1	−67.9 (11)	O40—Mo4—O26—Mo5	28.3 (8)
O20—Mo2—O15—Mo1	−130.7 (8)	O25—Mo4—O26—Mo5	−72.5 (4)
O21—Mo2—O15—Mo1	−58.3 (8)	O38—Mo4—O26—Mo5	85.2 (4)
O1—Mo1—O16—Mo7	168.2 (4)	O28—Mo4—O26—Mo5	1.6 (3)
O15—Mo1—O16—Mo7	−86.3 (4)	O6—Mo6—O27—Mo5	168.8 (4)
O13—Mo1—O16—Mo7	13.2 (8)	O29—Mo6—O27—Mo5	−84.0 (4)
O17—Mo1—O16—Mo7	70.2 (4)	O30—Mo6—O27—Mo5	12.9 (9)
O18—Mo1—O16—Mo7	−2.5 (3)	O25—Mo6—O27—Mo5	70.9 (4)
O7—Mo7—O16—Mo1	−174.4 (4)	O28—Mo6—O27—Mo5	−1.1 (3)
O32—Mo7—O16—Mo1	−71.7 (4)	O5—Mo5—O27—Mo6	−176.5 (4)
O38—Mo7—O16—Mo1	34.2 (8)	O37—Mo5—O27—Mo6	28.5 (9)
O31—Mo7—O16—Mo1	85.8 (4)	O26—Mo5—O27—Mo6	−73.5 (4)
O18—Mo7—O16—Mo1	2.5 (3)	O39—Mo5—O27—Mo6	84.0 (4)
O8—Mo8—O17—Mo1	169.6 (4)	O28—Mo5—O27—Mo6	1.1 (3)
O33—Mo8—O17—Mo1	−82.2 (4)	O18—P1—O28—Mo6	173.4 (3)
O37—Mo8—O17—Mo1	15.7 (8)	O24—P1—O28—Mo6	53.7 (5)
O32—Mo8—O17—Mo1	72.1 (4)	O21—P1—O28—Mo6	−66.8 (4)
O18—Mo8—O17—Mo1	0.2 (3)	O18—P1—O28—Mo5	52.9 (5)
O1—Mo1—O17—Mo8	−176.0 (4)	O24—P1—O28—Mo5	−66.8 (5)
O15—Mo1—O17—Mo8	25.9 (9)	O21—P1—O28—Mo5	172.7 (3)
O16—Mo1—O17—Mo8	−74.9 (4)	O18—P1—O28—Mo4	−66.4 (4)
O13—Mo1—O17—Mo8	83.3 (4)	O24—P1—O28—Mo4	173.9 (3)
O18—Mo1—O17—Mo8	−0.2 (3)	O21—P1—O28—Mo4	53.4 (5)
O28—P1—O18—Mo1	173.6 (3)	O6—Mo6—O28—P1	155.8 (13)
O24—P1—O18—Mo1	−66.6 (4)	O29—Mo6—O28—P1	−34.8 (4)
O21—P1—O18—Mo1	53.5 (5)	O27—Mo6—O28—P1	−135.0 (4)
O28—P1—O18—Mo7	53.6 (5)	O30—Mo6—O28—P1	51.0 (4)
O24—P1—O18—Mo7	173.4 (3)	O25—Mo6—O28—P1	133.7 (4)
O21—P1—O18—Mo7	−66.5 (5)	O6—Mo6—O28—Mo5	−68.4 (14)

O28—P1—O18—Mo8	−65.9 (5)	O29—Mo6—O28—Mo5	100.9 (2)
O24—P1—O18—Mo8	53.9 (5)	O27—Mo6—O28—Mo5	0.7 (2)
O21—P1—O18—Mo8	174.0 (3)	O30—Mo6—O28—Mo5	−173.2 (2)
O1—Mo1—O18—P1	160.2 (14)	O25—Mo6—O28—Mo5	−90.5 (2)
O15—Mo1—O18—P1	−34.0 (4)	O6—Mo6—O28—Mo4	20.8 (14)
O16—Mo1—O18—P1	−133.9 (4)	O29—Mo6—O28—Mo4	−169.8 (2)
O13—Mo1—O18—P1	53.0 (4)	O27—Mo6—O28—Mo4	90.0 (3)
O17—Mo1—O18—P1	135.8 (4)	O30—Mo6—O28—Mo4	−84.0 (2)
O1—Mo1—O18—Mo7	−64.2 (15)	O25—Mo6—O28—Mo4	−1.3 (2)
O15—Mo1—O18—Mo7	101.6 (2)	O5—Mo5—O28—P1	148.4 (14)
O16—Mo1—O18—Mo7	1.7 (2)	O37—Mo5—O28—P1	−34.0 (4)
O13—Mo1—O18—Mo7	−171.5 (2)	O26—Mo5—O28—P1	−133.4 (4)
O17—Mo1—O18—Mo7	−88.6 (2)	O27—Mo5—O28—P1	134.9 (5)
O1—Mo1—O18—Mo8	24.5 (16)	O39—Mo5—O28—P1	51.9 (4)
O15—Mo1—O18—Mo8	−169.7 (2)	O5—Mo5—O28—Mo6	12.8 (16)
O16—Mo1—O18—Mo8	90.4 (2)	O37—Mo5—O28—Mo6	−169.6 (2)
O13—Mo1—O18—Mo8	−82.7 (2)	O26—Mo5—O28—Mo6	91.0 (2)
O17—Mo1—O18—Mo8	0.1 (2)	O27—Mo5—O28—Mo6	−0.7 (2)
O32—Mo7—O18—P1	−133.1 (4)	O39—Mo5—O28—Mo6	−83.7 (2)
O38—Mo7—O18—P1	−32.8 (4)	O5—Mo5—O28—Mo4	−77.1 (15)
O16—Mo7—O18—P1	133.6 (4)	O37—Mo5—O28—Mo4	100.5 (2)
O31—Mo7—O18—P1	51.0 (4)	O26—Mo5—O28—Mo4	1.1 (2)
O32—Mo7—O18—Mo1	91.7 (2)	O27—Mo5—O28—Mo4	−90.6 (2)
O38—Mo7—O18—Mo1	−168.0 (2)	O39—Mo5—O28—Mo4	−173.6 (2)
O16—Mo7—O18—Mo1	−1.6 (2)	O4—Mo4—O28—P1	158.0 (13)
O31—Mo7—O18—Mo1	−84.2 (2)	O40—Mo4—O28—P1	−34.9 (4)
O32—Mo7—O18—Mo8	2.0 (2)	O25—Mo4—O28—P1	−134.0 (4)
O38—Mo7—O18—Mo8	102.3 (2)	O38—Mo4—O28—P1	50.7 (4)
O16—Mo7—O18—Mo8	−91.3 (2)	O26—Mo4—O28—P1	134.1 (4)
O31—Mo7—O18—Mo8	−173.9 (2)	O4—Mo4—O28—Mo6	−66.5 (15)
O8—Mo8—O18—P1	147.7 (13)	O40—Mo4—O28—Mo6	100.6 (2)
O33—Mo8—O18—P1	−33.9 (4)	O25—Mo4—O28—Mo6	1.4 (2)
O17—Mo8—O18—P1	−135.5 (5)	O38—Mo4—O28—Mo6	−173.8 (2)
O37—Mo8—O18—P1	51.5 (4)	O26—Mo4—O28—Mo6	−90.5 (2)
O32—Mo8—O18—P1	133.4 (4)	O4—Mo4—O28—Mo5	22.9 (15)
O8—Mo8—O18—Mo1	−76.9 (14)	O40—Mo4—O28—Mo5	−170.0 (2)
O33—Mo8—O18—Mo1	101.5 (2)	O25—Mo4—O28—Mo5	90.9 (2)
O17—Mo8—O18—Mo1	−0.1 (2)	O38—Mo4—O28—Mo5	−84.4 (2)
O37—Mo8—O18—Mo1	−173.1 (2)	O26—Mo4—O28—Mo5	−1.0 (2)
O32—Mo8—O18—Mo1	−91.1 (2)	O6—Mo6—O29—Mo10	−126.2 (7)
O8—Mo8—O18—Mo7	12.4 (15)	O27—Mo6—O29—Mo10	129.2 (7)
O33—Mo8—O18—Mo7	−169.2 (2)	O30—Mo6—O29—Mo10	−25.4 (7)
O17—Mo8—O18—Mo7	89.2 (2)	O25—Mo6—O29—Mo10	29.7 (12)
O37—Mo8—O18—Mo7	−83.8 (2)	O28—Mo6—O29—Mo10	55.8 (7)
O32—Mo8—O18—Mo7	−1.8 (2)	O10—Mo10—O29—Mo6	129.6 (7)
O2—Mo2—O19—Mo11	167.0 (4)	O35—Mo10—O29—Mo6	25.8 (7)
O14—Mo2—O19—Mo11	−86.1 (4)	O22—Mo10—O29—Mo6	−73.4 (10)
O20—Mo2—O19—Mo11	69.1 (4)	O34—Mo10—O29—Mo6	−133.8 (8)
O15—Mo2—O19—Mo11	7.7 (9)	O24—Mo10—O29—Mo6	−61.1 (7)

O21—Mo2—O19—Mo11	−2.2 (3)	O11—Mo11—O30—Mo6	−128.5 (7)
O11—Mo11—O19—Mo2	−174.8 (4)	O36—Mo11—O30—Mo6	125.4 (7)
O30—Mo11—O19—Mo2	32.0 (8)	O19—Mo11—O30—Mo6	24.2 (12)
O36—Mo11—O19—Mo2	−72.3 (4)	O35—Mo11—O30—Mo6	−28.6 (7)
O35—Mo11—O19—Mo2	85.6 (4)	O21—Mo11—O30—Mo6	52.3 (7)
O21—Mo11—O19—Mo2	2.2 (3)	O6—Mo6—O30—Mo11	133.1 (7)
O12—Mo12—O20—Mo2	168.7 (4)	O29—Mo6—O30—Mo11	28.9 (7)
O31—Mo12—O20—Mo2	−85.2 (4)	O27—Mo6—O30—Mo11	−71.0 (10)
O40—Mo12—O20—Mo2	14.0 (8)	O25—Mo6—O30—Mo11	−130.2 (8)
O36—Mo12—O20—Mo2	71.3 (4)	O28—Mo6—O30—Mo11	−57.3 (7)
O21—Mo12—O20—Mo2	−1.1 (3)	O12—Mo12—O31—Mo7	−131.9 (8)
O2—Mo2—O20—Mo12	−176.0 (4)	O20—Mo12—O31—Mo7	123.3 (8)
O14—Mo2—O20—Mo12	32.4 (8)	O40—Mo12—O31—Mo7	−30.4 (8)
O19—Mo2—O20—Mo12	−73.1 (4)	O36—Mo12—O31—Mo7	24.2 (13)
O15—Mo2—O20—Mo12	83.6 (4)	O21—Mo12—O31—Mo7	50.1 (8)
O21—Mo2—O20—Mo12	1.1 (3)	O7—Mo7—O31—Mo12	134.6 (8)
O18—P1—O21—Mo12	54.0 (5)	O32—Mo7—O31—Mo12	−64.3 (11)
O28—P1—O21—Mo12	−66.1 (5)	O38—Mo7—O31—Mo12	32.0 (8)
O24—P1—O21—Mo12	173.7 (3)	O16—Mo7—O31—Mo12	−127.5 (8)
O18—P1—O21—Mo2	−67.4 (5)	O18—Mo7—O31—Mo12	−55.0 (8)
O28—P1—O21—Mo2	172.4 (3)	O7—Mo7—O32—Mo8	167.6 (4)
O24—P1—O21—Mo2	52.2 (5)	O38—Mo7—O32—Mo8	−86.2 (4)
O18—P1—O21—Mo11	174.2 (3)	O16—Mo7—O32—Mo8	68.2 (4)
O28—P1—O21—Mo11	54.0 (5)	O31—Mo7—O32—Mo8	6.6 (8)
O24—P1—O21—Mo11	−66.2 (5)	O18—Mo7—O32—Mo8	−2.9 (3)
O12—Mo12—O21—P1	156.0 (13)	O8—Mo8—O32—Mo7	−174.4 (4)
O31—Mo12—O21—P1	−34.6 (4)	O33—Mo8—O32—Mo7	32.7 (8)
O20—Mo12—O21—P1	−135.4 (4)	O17—Mo8—O32—Mo7	−71.7 (4)
O40—Mo12—O21—P1	51.4 (4)	O37—Mo8—O32—Mo7	85.9 (4)
O36—Mo12—O21—P1	134.7 (4)	O18—Mo8—O32—Mo7	3.0 (3)
O12—Mo12—O21—Mo2	−67.9 (15)	O8—Mo8—O33—Mo9	−127.3 (8)
O31—Mo12—O21—Mo2	101.6 (2)	O17—Mo8—O33—Mo9	126.1 (8)
O20—Mo12—O21—Mo2	0.8 (2)	O37—Mo8—O33—Mo9	−27.3 (8)
O40—Mo12—O21—Mo2	−172.4 (2)	O32—Mo8—O33—Mo9	24.9 (12)
O36—Mo12—O21—Mo2	−89.1 (2)	O18—Mo8—O33—Mo9	53.0 (8)
O12—Mo12—O21—Mo11	21.2 (15)	O9—Mo9—O33—Mo8	131.8 (8)
O31—Mo12—O21—Mo11	−169.3 (2)	O39—Mo9—O33—Mo8	28.2 (8)
O20—Mo12—O21—Mo11	89.9 (2)	O34—Mo9—O33—Mo8	−73.2 (10)
O40—Mo12—O21—Mo11	−83.3 (2)	O23—Mo9—O33—Mo8	−130.9 (8)
O36—Mo12—O21—Mo11	0.03 (19)	O24—Mo9—O33—Mo8	−58.7 (8)
O2—Mo2—O21—P1	150.8 (13)	O9—Mo9—O34—Mo10	170.8 (4)
O14—Mo2—O21—P1	−31.6 (4)	O39—Mo9—O34—Mo10	−82.3 (4)
O19—Mo2—O21—P1	−132.3 (5)	O33—Mo9—O34—Mo10	15.6 (8)
O20—Mo2—O21—P1	135.5 (5)	O23—Mo9—O34—Mo10	72.2 (4)
O15—Mo2—O21—P1	52.2 (4)	O24—Mo9—O34—Mo10	0.7 (3)
O2—Mo2—O21—Mo12	14.6 (15)	O10—Mo10—O34—Mo9	−176.7 (4)
O14—Mo2—O21—Mo12	−167.8 (2)	O35—Mo10—O34—Mo9	24.5 (8)
O19—Mo2—O21—Mo12	91.5 (3)	O22—Mo10—O34—Mo9	−75.2 (4)
O20—Mo2—O21—Mo12	−0.7 (2)	O29—Mo10—O34—Mo9	81.4 (4)

O15—Mo2—O21—Mo12	−84.0 (2)	O24—Mo10—O34—Mo9	−0.7 (3)
O2—Mo2—O21—Mo11	−75.5 (15)	O10—Mo10—O35—Mo11	−128.9 (7)
O14—Mo2—O21—Mo11	102.1 (2)	O22—Mo10—O35—Mo11	126.4 (7)
O19—Mo2—O21—Mo11	1.4 (2)	O29—Mo10—O35—Mo11	−26.6 (7)
O20—Mo2—O21—Mo11	−90.8 (2)	O34—Mo10—O35—Mo11	29.5 (12)
O15—Mo2—O21—Mo11	−174.1 (2)	O24—Mo10—O35—Mo11	53.4 (7)
O11—Mo11—O21—P1	149.9 (13)	O11—Mo11—O35—Mo10	131.6 (7)
O30—Mo11—O21—P1	−34.3 (4)	O30—Mo11—O35—Mo10	28.0 (7)
O36—Mo11—O21—P1	−135.5 (5)	O36—Mo11—O35—Mo10	−72.7 (10)
O19—Mo11—O21—P1	133.0 (5)	O19—Mo11—O35—Mo10	−131.2 (8)
O35—Mo11—O21—P1	50.8 (4)	O21—Mo11—O35—Mo10	−58.9 (7)
O11—Mo11—O21—Mo12	−74.6 (15)	O11—Mo11—O36—Mo12	169.8 (3)
O30—Mo11—O21—Mo12	101.1 (2)	O30—Mo11—O36—Mo12	−83.0 (4)
O36—Mo11—O21—Mo12	0.0 (2)	O19—Mo11—O36—Mo12	71.4 (4)
O19—Mo11—O21—Mo12	−91.5 (2)	O35—Mo11—O36—Mo12	14.2 (8)
O35—Mo11—O21—Mo12	−173.8 (2)	O21—Mo11—O36—Mo12	0.0 (3)
O11—Mo11—O21—Mo2	15.6 (16)	O12—Mo12—O36—Mo11	−176.1 (4)
O30—Mo11—O21—Mo2	−168.7 (2)	O31—Mo12—O36—Mo11	27.4 (8)
O36—Mo11—O21—Mo2	90.1 (2)	O20—Mo12—O36—Mo11	−74.7 (4)
O19—Mo11—O21—Mo2	−1.3 (2)	O40—Mo12—O36—Mo11	82.8 (4)
O35—Mo11—O21—Mo2	−83.6 (2)	O21—Mo12—O36—Mo11	0.0 (3)
O10—Mo10—O22—Mo3	167.9 (4)	O5—Mo5—O37—Mo8	−126.5 (7)
O35—Mo10—O22—Mo3	−85.4 (4)	O26—Mo5—O37—Mo8	127.5 (7)
O29—Mo10—O22—Mo3	10.8 (8)	O27—Mo5—O37—Mo8	28.0 (12)
O34—Mo10—O22—Mo3	70.3 (4)	O39—Mo5—O37—Mo8	−26.6 (7)
O24—Mo10—O22—Mo3	−1.8 (3)	O28—Mo5—O37—Mo8	53.9 (7)
O3—Mo3—O22—Mo10	−174.4 (4)	O8—Mo8—O37—Mo5	131.5 (7)
O23—Mo3—O22—Mo10	−72.1 (4)	O33—Mo8—O37—Mo5	27.0 (7)
O13—Mo3—O22—Mo10	28.2 (8)	O17—Mo8—O37—Mo5	−74.4 (10)
O14—Mo3—O22—Mo10	85.1 (4)	O32—Mo8—O37—Mo5	−132.2 (8)
O24—Mo3—O22—Mo10	1.9 (3)	O18—Mo8—O37—Mo5	−59.3 (7)
O3—Mo3—O23—Mo9	166.9 (4)	O7—Mo7—O38—Mo4	−131.9 (8)
O13—Mo3—O23—Mo9	−86.8 (4)	O32—Mo7—O38—Mo4	122.6 (8)
O22—Mo3—O23—Mo9	68.3 (4)	O16—Mo7—O38—Mo4	19.1 (12)
O14—Mo3—O23—Mo9	4.7 (9)	O31—Mo7—O38—Mo4	−31.8 (8)
O24—Mo3—O23—Mo9	−3.1 (3)	O18—Mo7—O38—Mo4	49.0 (8)
O9—Mo9—O23—Mo3	−172.1 (4)	O4—Mo4—O38—Mo7	135.1 (8)
O39—Mo9—O23—Mo3	31.6 (8)	O40—Mo4—O38—Mo7	31.5 (8)
O34—Mo9—O23—Mo3	−71.6 (4)	O25—Mo4—O38—Mo7	−65.6 (11)
O33—Mo9—O23—Mo3	86.2 (4)	O26—Mo4—O38—Mo7	−127.7 (8)
O24—Mo9—O23—Mo3	3.2 (3)	O28—Mo4—O38—Mo7	−54.9 (8)
O18—P1—O24—Mo10	173.7 (3)	O9—Mo9—O39—Mo5	−129.3 (7)
O28—P1—O24—Mo10	−66.3 (5)	O34—Mo9—O39—Mo5	126.5 (7)
O21—P1—O24—Mo10	54.1 (5)	O33—Mo9—O39—Mo5	−27.1 (7)
O18—P1—O24—Mo3	53.7 (5)	O23—Mo9—O39—Mo5	26.5 (12)
O28—P1—O24—Mo3	173.7 (3)	O24—Mo9—O39—Mo5	53.3 (7)
O21—P1—O24—Mo3	−66.0 (5)	O5—Mo5—O39—Mo9	131.5 (8)
O18—P1—O24—Mo9	−66.8 (4)	O37—Mo5—O39—Mo9	28.0 (8)
O28—P1—O24—Mo9	53.2 (5)	O26—Mo5—O39—Mo9	−70.5 (10)

O21—P1—O24—Mo9	173.6 (3)	O27—Mo5—O39—Mo9	−131.7 (8)
O10—Mo10—O24—P1	157.3 (13)	O28—Mo5—O39—Mo9	−58.8 (7)
O35—Mo10—O24—P1	−34.5 (4)	O4—Mo4—O40—Mo12	−126.7 (7)
O22—Mo10—O24—P1	−134.3 (4)	O25—Mo4—O40—Mo12	128.7 (7)
O29—Mo10—O24—P1	51.6 (4)	O38—Mo4—O40—Mo12	−25.9 (7)
O34—Mo10—O24—P1	135.3 (5)	O26—Mo4—O40—Mo12	30.3 (12)
O10—Mo10—O24—Mo3	−67.2 (15)	O28—Mo4—O40—Mo12	55.6 (7)
O35—Mo10—O24—Mo3	101.0 (2)	O12—Mo12—O40—Mo4	129.8 (7)
O22—Mo10—O24—Mo3	1.2 (2)	O31—Mo12—O40—Mo4	26.9 (7)
O29—Mo10—O24—Mo3	−172.9 (2)	O20—Mo12—O40—Mo4	−75.5 (10)
O34—Mo10—O24—Mo3	−89.2 (2)	O36—Mo12—O40—Mo4	−133.7 (8)
O10—Mo10—O24—Mo9	22.5 (15)	O21—Mo12—O40—Mo4	−60.8 (7)
O35—Mo10—O24—Mo9	−169.4 (2)	C2—N3—C1—N1	−159.0 (10)
O22—Mo10—O24—Mo9	90.9 (2)	C2—N3—C1—N2	20.0 (15)
O29—Mo10—O24—Mo9	−83.2 (2)	C8—N5—C2—N4	2.6 (10)
O34—Mo10—O24—Mo9	0.5 (2)	C8—N5—C2—N3	−171.1 (8)
O3—Mo3—O24—P1	155.3 (14)	C3—N4—C2—N5	−1.7 (10)
O23—Mo3—O24—P1	−133.2 (4)	C3—N4—C2—N3	171.3 (9)
O13—Mo3—O24—P1	−35.0 (4)	C1—N3—C2—N5	−149.1 (9)
O22—Mo3—O24—P1	134.1 (4)	C1—N3—C2—N4	38.3 (15)
O14—Mo3—O24—P1	50.1 (4)	C2—N4—C3—C8	0.2 (10)
O3—Mo3—O24—Mo10	20.0 (16)	C2—N4—C3—C4	−178.1 (9)
O23—Mo3—O24—Mo10	91.5 (2)	C8—C3—C4—C5	0.3 (13)
O13—Mo3—O24—Mo10	−170.3 (2)	N4—C3—C4—C5	178.4 (9)
O22—Mo3—O24—Mo10	−1.1 (2)	C3—C4—C5—C6	−2.2 (14)
O14—Mo3—O24—Mo10	−85.1 (2)	C4—C5—C6—C7	1.9 (16)
O3—Mo3—O24—Mo9	−69.4 (16)	C5—C6—C7—C8	0.3 (15)
O23—Mo3—O24—Mo9	2.1 (2)	C6—C7—C8—C3	−2.2 (14)
O13—Mo3—O24—Mo9	100.3 (2)	C6—C7—C8—N5	−179.4 (9)
O22—Mo3—O24—Mo9	−90.5 (2)	C4—C3—C8—C7	2.0 (14)
O14—Mo3—O24—Mo9	−174.5 (2)	N4—C3—C8—C7	−176.5 (8)
O9—Mo9—O24—P1	159.7 (12)	C4—C3—C8—N5	179.8 (8)
O39—Mo9—O24—P1	−34.2 (4)	N4—C3—C8—N5	1.3 (9)
O34—Mo9—O24—P1	−135.5 (5)	C2—N5—C8—C7	175.2 (9)
O33—Mo9—O24—P1	51.2 (4)	C2—N5—C8—C3	−2.3 (10)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O4^{i}	0.96	2.14	3.097 (9)	173
O8—H8···O10^{ii}	0.96	2.40	3.093 (5)	129
N1—H1N1···O5S^{iii}	0.88	1.95	2.728 (6)	146
N1—H2N1···O5W^{iv}	0.88	2.20	2.883 (6)	134
N2—H1N2···O5S^{iii}	0.88	2.10	2.839 (6)	141
N2—H2N2···O5	0.88	2.01	2.844 (6)	157
N3—H1N3···O1W	0.90	1.84	2.717 (6)	165
N5—H1N5···O36^{ii}	0.90	2.25	2.974 (5)	137
O1S—H1OS···O32	0.95	2.35	3.218 (5)	152

O3S—H3OS···O5W^{v}	0.96	2.01	2.881 (7)	149
O4S—H4OS···O27	0.96	1.99	2.805 (6)	141
O1W—H1W1···O20^{ii}	1.01	1.89	2.740 (6)	140
O1W—H2W1···O5W'^{iv}	1.01	2.05	3.057 (7)	176
O1W—H2W1···O5W^{iv}	1.01	2.17	3.067 (7)	148
O2W—H2W2···N4	1.01	1.78	2.731 (6)	157
O3W—H2W3···O3S	1.01	1.93	2.618 (8)	123
O4W—H1W4···O6^{ii}	1.01	2.30	3.004 (7)	126
O4W—H2W4···O2S	1.01	1.76	2.716 (7)	157
O5W—H4W'···O32^{vi}	1.01	1.87	2.847 (7)	161

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

Fig. 1

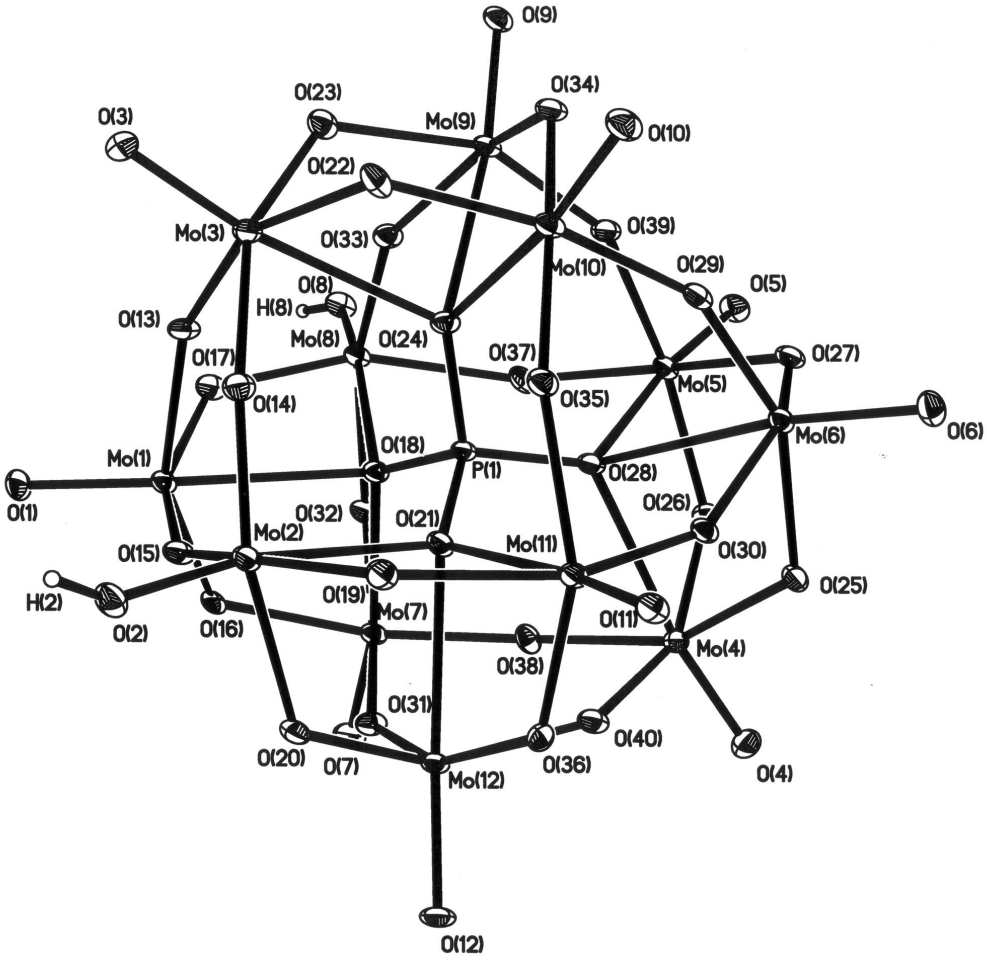
O(9)
O(23)
O(34)
O(3)
Mo(9)
O(10)
O(22)
O(39)
Mo(3)
O(33)
Mo(10)
O(29)
O(5)
O(8)
H(8)
O(13)
Mo(8)
O(24)
O(37)
O(27)
O(17)
O(14)
O(35)
Mo(5)
Mo(6)
O(6)
Mo(1)
O(18)
P(1)
O(28)
O(1)
O(32)
O(21)
O(26)
Mo(2)
Mo(11)
O(15)
O(30)
O(19)
O(25)
H(2)
Mo(7)
O(11)
O(2)
O(16)
O(38)
Mo(4)
O(31)
O(40)
O(20)
O(7)
O(36)
O(4)
Mo(12)
O(12)

Fig. 2

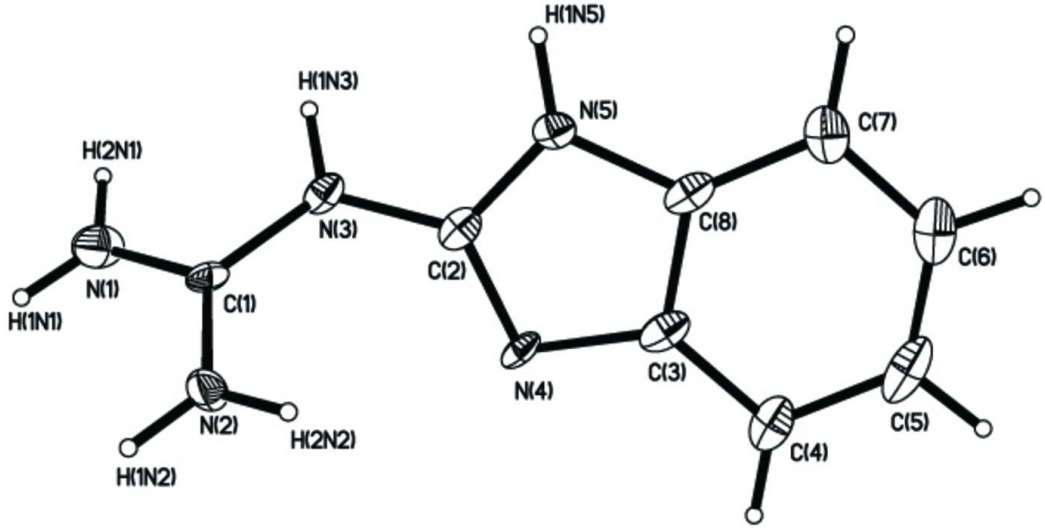
H(1N5)
H(1N3)
N(5)
C(7)
H(2N1)
N(3)
C(8)
C(6)
C(2)
N(1)
C(1)
H(1N1)
N(4)
C(3)
C(5)
N(2)
H(2N2)
C(4)
H(1N2)

Fig. 3

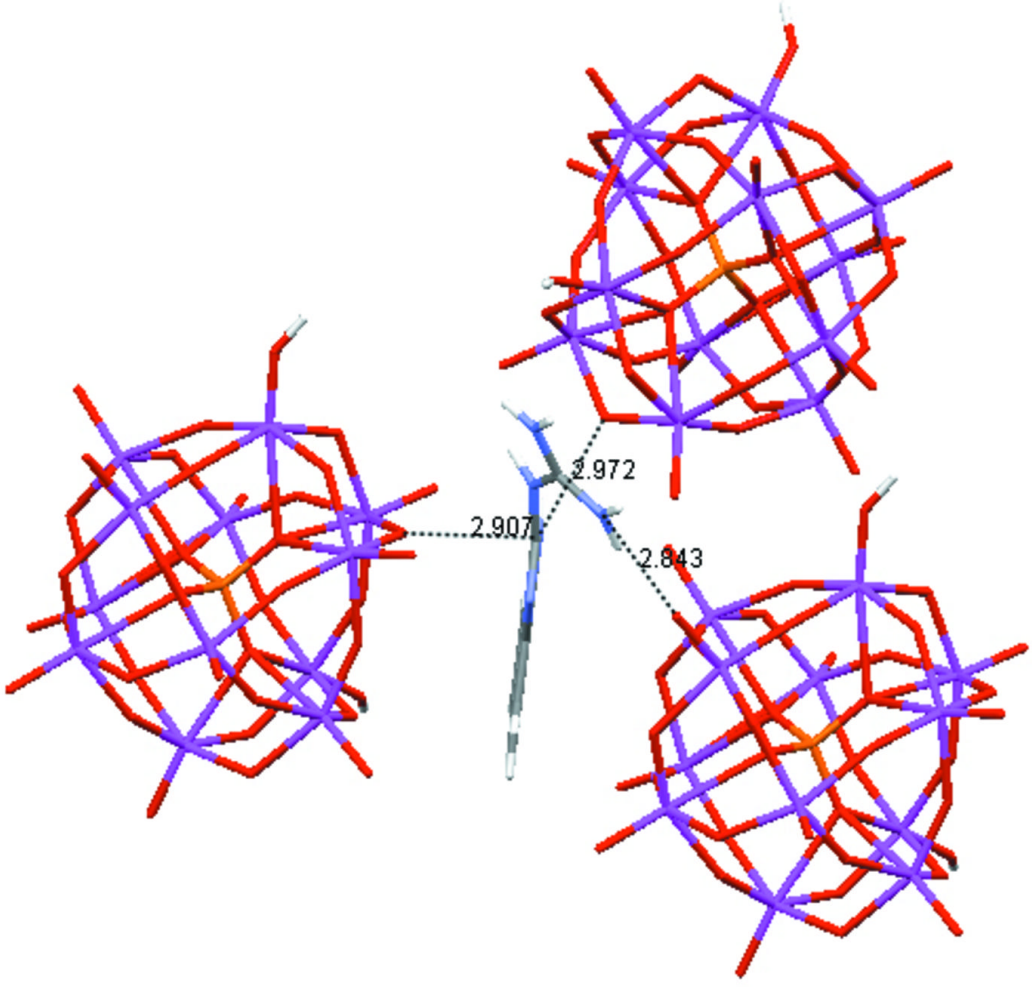

Fig. 4

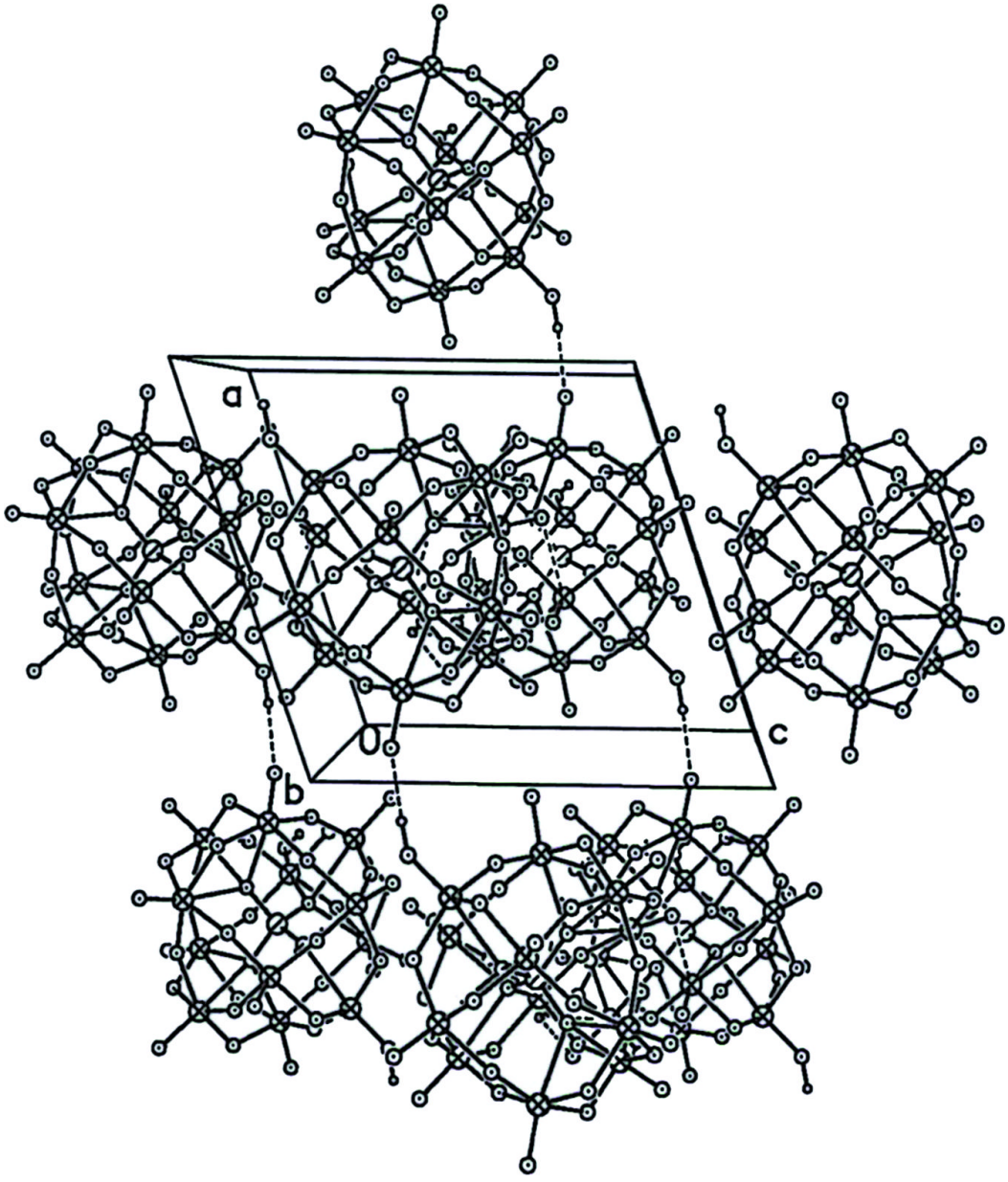

Fig. 5

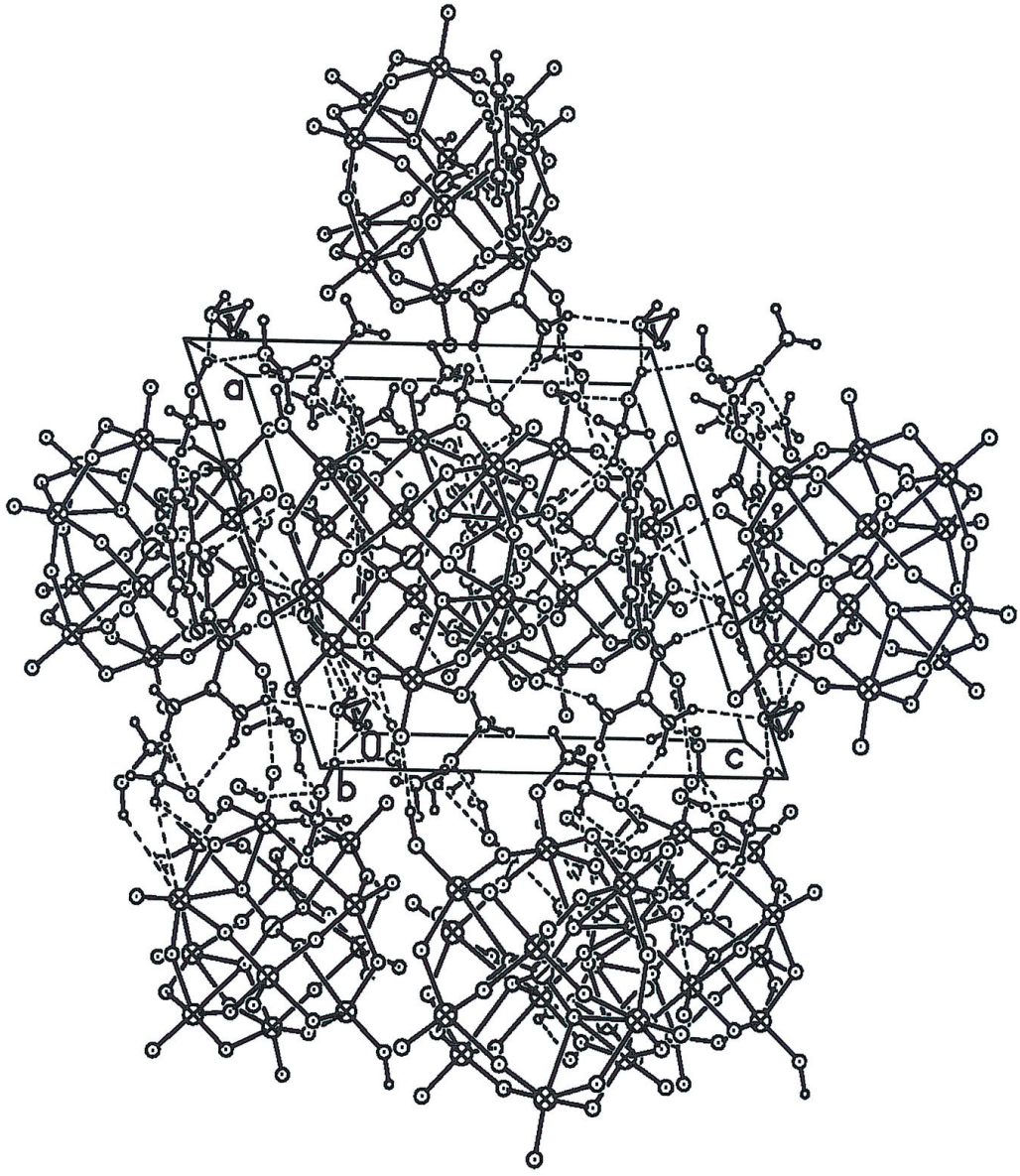

Fig. 6