



Crystal structure of octakis(*N,N*-dimethylformamide- κ O)europium(III) tetracosam μ_2 -oxido-dodecaoxido- μ_{12} -phosphato-dodecamolybdate(VI)

Yassine Ghandour,^{a*} Imen Hammami,^a Shabir Najmudin,^b Cecilia Bonifácio^c and Mohamed Salah Belkhiria^a

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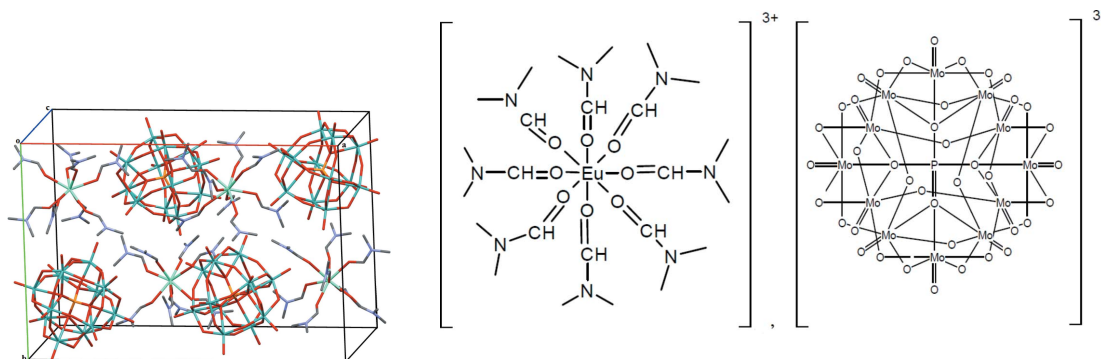
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^aLaboratoire de Physico-chimie des Matériaux, Faculté des Sciences de Monastir, Avenue de l'environnement, 5019 Monastir, University of Monastir, Tunisia, ^bFaculdade de Medicina, Veterinária, Universidade Tecnica de Lisboa, Avenida da Universidade Tecnica, 1300-477 Lisboa, Portugal, and ^cREQUIMTE/CQFB Departamento de Quimica, Faculdade de Ciencias e Tecnologia, Universidade Nova de Lisboa, 2829-516 Caparica, Portugal. *Correspondence e-mail: ghandour_yassine@hotmail.fr

In the title salt, [Eu(C₃H₇NO)₈][PMo₁₂O₄₀], the asymmetric unit comprises one α -Keggin-type [PMo₁₂O₄₀]³⁻ polyoxidometalate anion and one distorted dodecahedral [Eu(C₃H₇NO)₈]³⁺ complex cation. In the crystal, the isolated polyoxidometalate anions are packed into hexagonally arranged rows extending parallel to [001]. The complex cations are situated between the rows and are linked to the neighbouring anions through weak C—H...O hydrogen-bonding interactions, leading to the formation of a three-dimensional network structure.

1. Chemical context

Polyoxidometalates (POMs) are versatile metal–oxygen complexes which have attracted interest due to their topological properties and their potential applications in catalysis, photoluminescence, electrochromism and magnetism (Long *et al.*, 2010; Pope & Müller, 2010; Coronado & Gómez-García, 1998). Up to date, a variety of strategies have been developed and used to assemble POM-based hybrid materials by controlling reaction factors such as metal ions, organic ligands, POM species, pH, molar ratio of raw materials or reaction environments (Wang *et al.*, 2013; Liu *et al.*, 2013). Even with these approaches, the design and synthesis of new stable polyoxidomolybdate complexes are still challenging.



Herein, we report on the synthesis, UV–vis and IR spectra along with the crystal structure of the hybrid europium(III) POM title compound, [Eu(C₃H₇NO)₈][PMo₁₂O₄₀], (I).

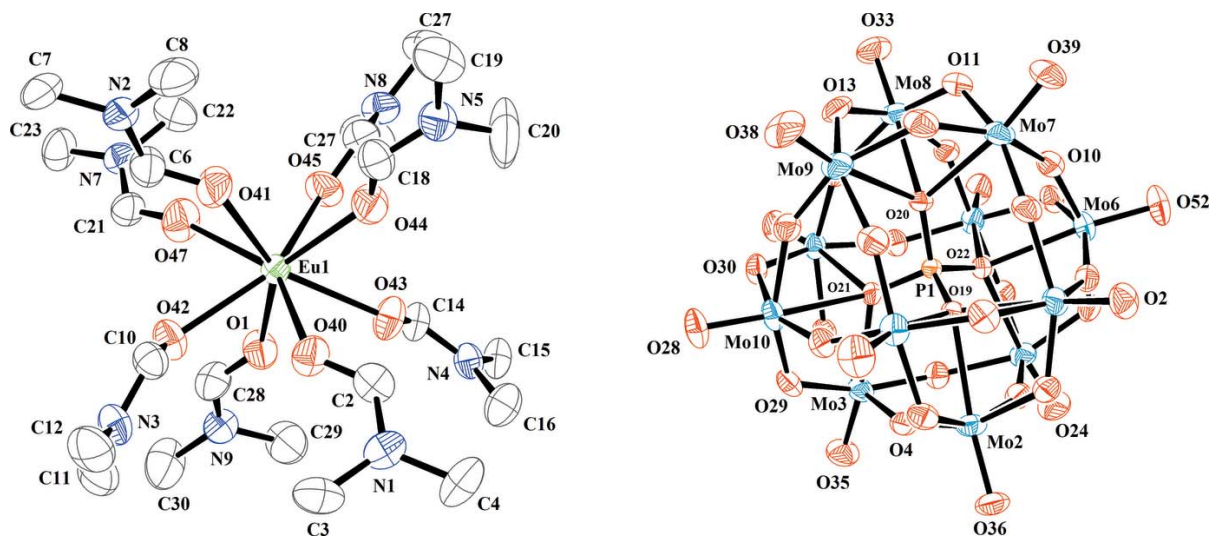


Figure 1
The molecular structures of the cation and anion in compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 40% probability level. H atoms have been omitted for clarity.

2. Structural commentary

The structures of the molecular components of compound (I) are illustrated in Fig. 1. The $[\text{PMo}_{12}\text{O}_{40}]^{3-}$ polyoxidoanion of (I) exhibits a classical α -Keggin-type structure. The central P atom is tetrahedrally surrounded with all four oxygen atoms (O_a) linked to four Mo_3O_{13} moieties. The latter species are fused together by sharing corner atoms (O_b) and consist of three MoO_6 octahedra condensed in a triangular arrangement by sharing edges (O_c). There is also a terminal oxygen atom (O_d) in every MoO_6 octahedron. The P–O bond lengths range from 1.521 (5) Å to 1.536 (4) Å and the Mo–O bond lengths from 1.690 (5) Å to 2.438 (4) Å. The O–P–O angles [109.1 (2)–109.8 (3)°] indicate only a slight distortion of the central PO_4 tetrahedron. The Eu^{III} cation is coordinated by eight dimethylformamide ligands through their oxygen atoms

with Eu–O distances from 2.369 (5) to 2.416 (6) Å. These values are comparable to those of related oxido-europium(III) species, *e.g.* for the $[\text{Eu}(\text{thd})_3(\text{DMF})_2]$ complex (thd is the ion of 2,2,6,6-tetramethyl-3,5-heptanedione) with Eu–O = 2.494 (5)–2.442 (5) Å (Cunningham & Siever, 1980). Calculations with the *SHAPE* software (Alvarez *et al.*, 2005) indicate that the coordination polyhedron of Eu^{III} is a slightly distorted dodecahedron approaching molecular D_{2d} symmetry (Casanova *et al.*, 2005).

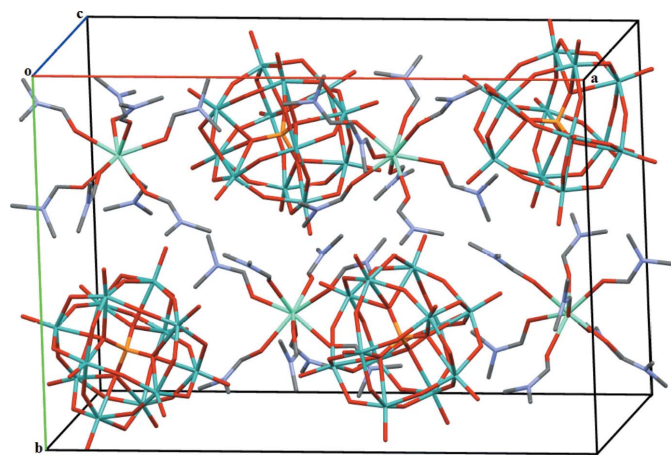


Figure 2
The contents of the unit cell of complex (I). H atoms have been omitted for clarity.

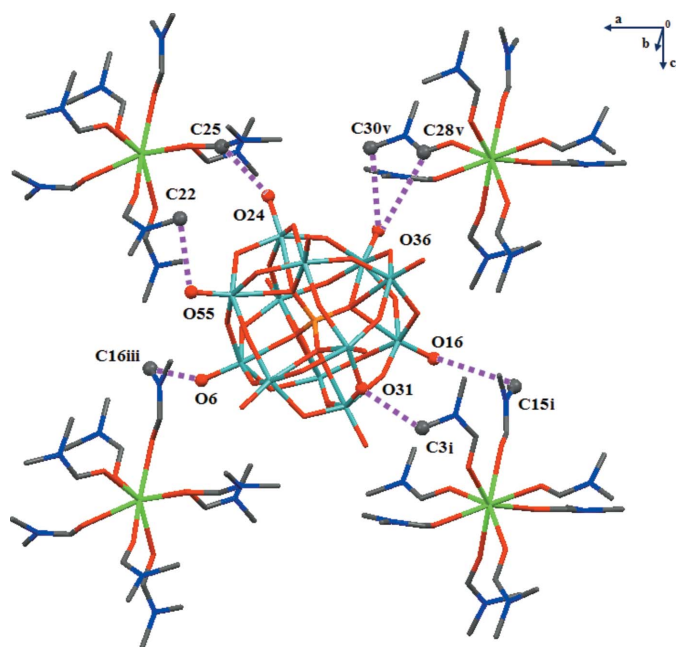


Figure 3
C–H...O hydrogen bonds (dashed lines) link one $[\text{Eu}(\text{dmf})_8]^{3+}$ cation to four neighbouring α -Keggin-type $[\text{PMo}_{12}\text{O}_{40}]^{3-}$ anions. Symmetry codes refer to Table 1.

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

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------------|-------|-------------|-------------|---------------|
| C3—H4···O31 ⁱ | 0.96 | 2.72 | 3.289 (11) | 118 |
| C4—H7···O36 ⁱⁱ | 0.96 | 2.61 | 3.476 (12) | 150 |
| C7—H13···O7 | 0.96 | 2.65 | 3.473 (12) | 145 |
| C8—H15···O28 ⁱⁱ | 0.96 | 2.51 | 3.316 (13) | 141 |
| C8—H16···O5 | 0.96 | 2.58 | 3.424 (11) | 147 |
| C10—H18···O28 ⁱⁱ | 0.93 | 2.62 | 3.516 (10) | 162 |
| C15—H29···O16 ⁱ | 0.96 | 2.55 | 3.299 (12) | 135 |
| C15—H27···O32 ⁱⁱⁱ | 0.96 | 2.52 | 3.440 (10) | 160 |
| C15—H28···O52 ^{iv} | 0.96 | 2.29 | 3.174 (10) | 153 |
| C16—H31···O6 ⁱⁱⁱ | 0.96 | 2.63 | 3.541 (11) | 159 |
| C22—H41···O55 | 0.96 | 2.53 | 3.280 (12) | 135 |
| C22—H42···O11 ^{iv} | 0.96 | 2.45 | 3.305 (11) | 149 |
| C22—H43···O45 | 0.96 | 2.61 | 3.567 (13) | 172 |
| C23—H44···O17 ^v | 0.96 | 2.52 | 3.443 (11) | 161 |
| C25—H55···O24 | 0.93 | 2.53 | 3.337 (11) | 145 |
| C25—H55···O44 | 0.93 | 2.58 | 3.091 (10) | 115 |
| C28—H56···O36 ^v | 0.93 | 2.62 | 3.476 (11) | 153 |
| C30—H60···O36 ^v | 0.96 | 2.58 | 3.458 (14) | 152 |

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

3. Supramolecular features

The unit cell content of the title compound is illustrated in Fig. 2. In the crystal structure of (I), each $[\text{Eu}(\text{DMF})_8]^{3+}$ cation is linked to four neighbouring α -Keggin-type $[\text{PMo}_{12}\text{O}_{40}]^{3-}$ anions through C—H···O hydrogen-bonding interactions between the methyl groups of the DMF ligands and the terminal-oxygen (O_d) and the bridging-oxygen atoms ($\text{O}_{b,c}$) of the $[\text{PMo}_{12}\text{O}_{40}]^{3-}$ anions (Fig. 3, Table 1). The C(donor)···O_d(acceptor) distances are between 3.174 (10) and 3.541 (11) Å while the C···O_(b,c) distances are between 3.289 (11) and 3.473 (12) Å. In the crystal packing, the POM anions are packed into hexagonally arranged rows extending parallel to [001] with the $[\text{Eu}(\text{DMF})_8]^{3+}$ cations located between the rows (Fig. 4).

4. Synthesis and crystallization

The starting material $[(\text{C}_4\text{H}_9)_4\text{N}]_4\text{H}_3[\text{PMo}_{11}\text{O}_{39}]$ was prepared using a literature method (Combs-Walker & Hill, 1998). $\text{EuCl}_3 \cdot 6\text{H}_2\text{O}$ (361.41 mg, 1 mmol) and isonicotinic acid

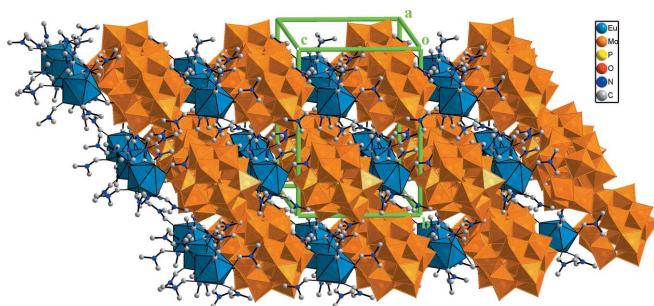


Figure 4
 The crystal packing of (I) with the $[\text{PMo}_{12}\text{O}_{40}]^{3-}$ anions in polyhedral representation.

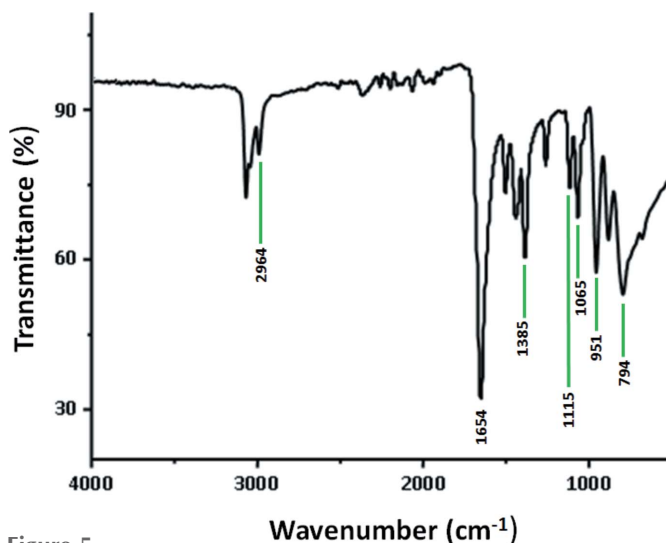


Figure 5
 The FT-IR spectrum of (I).

($\text{C}_6\text{H}_5\text{NO}_2$) (123.11 mg, 1 mmol) were dissolved in 10 ml of dimethylformamide. This solution was added dropwise to a yellow dimethylformamide solution of $[(\text{C}_4\text{H}_9)_4\text{N}]_4\text{H}_3[\text{PMo}_{11}\text{O}_{39}]$ (0.33 mmol in 10 ml). The mixture was heated under stirring for 1 h at 333 K. Single crystals of the title compounds were obtained by slow diffusion of 2-propanol through the dimethylformamide solution. UV-vis spectrum in dimethylformamide: λ_{max} (nm) 315 and 205.

5. FT-IR spectroscopy

The FT-IR spectrum was recorded in the range 4000–400 cm^{-1} on a Nicolet 470 FT-IR spectrophotometer with pressed KBr pellets.

The FT-IR spectrum of (I) (Fig. 5) exhibits characteristic bands attributed to the stretching and deformation modes of the Mo—O bond vibration of the $[\text{PMo}_{12}\text{O}_{40}]^{3-}$ anion in the region 1100–400 cm^{-1} . Thus, the asymmetric vibration $\nu_{\text{as}}(\text{P}-\text{O}_a)$, $\nu_{\text{as}}(\text{Mo}=\text{O}_d)$, $\nu_{\text{as}}(\text{Mo}-\text{O}_b-\text{Mo})$ and $\nu_{\text{as}}(\text{Mo}-\text{O}_c-\text{Mo})$ appear at 1065, 951, 885 and 974 cm^{-1} , respectively (Masteri-Farahani & Shahbazi, 2012). The absorption bands at 1265 and 1657 cm^{-1} are characteristic of the asymmetric vibration of the C—N and the C=O bonds, respectively. The vibration bands at 1115, 1440, 1385 and 2964 cm^{-1} are attributed to the vibration $\rho(\text{CH}_3)$ (rocking vibration), $\delta_a(\text{CH}_3)$, $\delta_s(\text{CH}_3)$ and $\nu(\text{C}-\text{H})$ of the dimethylformamide ligand (Durgaprasad *et al.*, 1971).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were placed in calculated positions and refined as riding atoms: C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for methine groups and C—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl groups. The refined Flack parameter (Parsons *et al.*, 2013) of -0.015 (7) indicates the correct determination of the absolute structure.

Table 2

Experimental details.

| | |
|--|--|
| Crystal data | |
| Chemical formula | [Eu(C ₃ H ₇ NO) ₈][PMo ₁₂ O ₄₀] |
| <i>M_r</i> | 2558.97 |
| Crystal system, space group | Orthorhombic, <i>Pna</i> 2 ₁ |
| Temperature (K) | 296 |
| <i>a</i> , <i>b</i> , <i>c</i> (Å) | 26.9108 (10), 18.3506 (6), 13.4494 (4) |
| <i>V</i> (Å ³) | 6641.7 (4) |
| <i>Z</i> | 4 |
| Radiation type | Mo <i>K</i> α |
| μ (mm ⁻¹) | 3.24 |
| Crystal size (mm) | 0.20 × 0.18 × 0.17 |
| Data collection | |
| Diffraction | Bruker APEXII CCD |
| Absorption correction | Multi-scan (<i>SADABS</i> ; Bruker, 2006) |
| <i>T</i> _{min} , <i>T</i> _{max} | 0.667, 0.747 |
| No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections | 88354, 33285, 19583 |
| <i>R</i> _{int} | 0.075 |
| (sin θ/λ) _{max} (Å ⁻¹) | 0.849 |
| Refinement | |
| <i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i> | 0.047, 0.095, 0.98 |
| No. of reflections | 33285 |
| No. of parameters | 863 |
| No. of restraints | 1 |
| H-atom treatment | H-atom parameters constrained |
| Δρ _{max} , Δρ _{min} (e Å ⁻³) | 2.08, -1.80 |
| Absolute structure | Flack <i>x</i> determined using 6924 quotients [(<i>I</i> ⁺) - (<i>I</i> ⁻)] / [(<i>I</i> ⁺) + (<i>I</i> ⁻)] |
| Absolute structure parameter | -0.015 (7) |

Computer programs: *APEX2* and *SAINT* (Bruker, 2006), *SIR2004* (Burla *et al.*, 2005), *SHELXL2014* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *DIAMOND* (Putz & Brandenburg, 2014) and *WinGX* (Farrugia, 2012).

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Crystal structure of octakis(*N,N*-dimethylformamide- κ O)europium(III) tetracosa- μ_2 -oxido-dodecaoxido- μ_{12} -phosphato-dodecamolybdate(VI)

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Computing details

Data collection: *APEX2* (Bruker, 2006); cell refinement: *SAINT* (Bruker, 2006); data reduction: *SAINT* (Bruker, 2006); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *DIAMOND* (Putz & Brandenburg, 2014); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

Octakis(*N,N*-dimethylformamide- κ O)europium(III) tetracosa- μ_2 -oxido-dodecaoxido- μ_{12} -phosphato-dodecamolybdate(VI)

Crystal data

[Eu(C₃H₇NO)₈][PMo₁₂O₄₀]

$M_r = 2558.97$

Orthorhombic, *Pna*2₁

$a = 26.9108$ (10) Å

$b = 18.3506$ (6) Å

$c = 13.4494$ (4) Å

$V = 6641.7$ (4) Å³

$Z = 4$

$F(000) = 4888$

$D_x = 2.559$ Mg m⁻³

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

Cell parameters from 9528 reflections

$\theta = 3.0$ – 32.3°

$\mu = 3.24$ mm⁻¹

$T = 296$ K

Prism, yellow

$0.20 \times 0.18 \times 0.17$ mm

Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2006)

$T_{\min} = 0.667$, $T_{\max} = 0.747$

88354 measured reflections

33285 independent reflections

19583 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.075$

$\theta_{\max} = 37.1^\circ$, $\theta_{\min} = 2.2^\circ$

$h = -41 \rightarrow 45$

$k = -31 \rightarrow 31$

$l = -21 \rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.047$

$wR(F^2) = 0.095$

$S = 0.98$

33285 reflections

863 parameters

1 restraint

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

$$w = 1/[\sigma^2(F_o^2) + (0.035P)^2]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

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

$$\Delta\rho_{\max} = 2.08 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.80 \text{ e } \text{\AA}^{-3}$$

Absolute structure: Flack x determined using

$$6924 \text{ quotients } [(I^+)-(I^-)]/[(I^+)+(I^-)]$$

Absolute structure parameter: -0.015 (7)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|--------------|-------------|--------------|----------------------------------|
| Eu1 | 0.62226 (2) | 0.24667 (2) | 0.27301 (3) | 0.03117 (7) |
| Mo1 | 0.26680 (2) | 0.18597 (3) | 0.63650 (5) | 0.03332 (13) |
| Mo2 | 0.30169 (2) | 0.35458 (3) | 0.55755 (5) | 0.03366 (13) |
| Mo3 | 0.41829 (3) | 0.43690 (3) | 0.64996 (5) | 0.03387 (13) |
| Mo4 | 0.47559 (2) | 0.36195 (3) | 0.85122 (5) | 0.03004 (12) |
| Mo5 | 0.49335 (2) | 0.20234 (3) | 0.68682 (5) | 0.03324 (13) |
| Mo6 | 0.39245 (3) | 0.10613 (3) | 0.60967 (5) | 0.03505 (14) |
| Mo7 | 0.32991 (3) | 0.10420 (3) | 0.85410 (5) | 0.03838 (15) |
| Mo8 | 0.43839 (3) | 0.17833 (4) | 0.93808 (5) | 0.03661 (14) |
| Mo9 | 0.32843 (3) | 0.26018 (4) | 0.99282 (5) | 0.04260 (17) |
| Mo10 | 0.36044 (2) | 0.43617 (3) | 0.87490 (5) | 0.03517 (14) |
| Mo11 | 0.25072 (2) | 0.33286 (4) | 0.78760 (5) | 0.03541 (14) |
| Mo12 | 0.42166 (3) | 0.26738 (4) | 0.49994 (5) | 0.03432 (13) |
| P1 | 0.37299 (6) | 0.26883 (8) | 0.74508 (12) | 0.0207 (3) |
| O1 | 0.6764 (2) | 0.1551 (4) | 0.2093 (5) | 0.0526 (16) |
| O2 | 0.2228 (2) | 0.1295 (3) | 0.5946 (5) | 0.0453 (14) |
| O3 | 0.26515 (19) | 0.2607 (3) | 0.5440 (4) | 0.0350 (11) |
| O4 | 0.34964 (18) | 0.4169 (3) | 0.6033 (4) | 0.0320 (10) |
| O5 | 0.47195 (19) | 0.4273 (3) | 0.7347 (4) | 0.0325 (11) |
| O6 | 0.5310 (2) | 0.3873 (3) | 0.8969 (4) | 0.0420 (13) |
| O7 | 0.49746 (19) | 0.2908 (3) | 0.7483 (4) | 0.0330 (11) |
| O8 | 0.45951 (19) | 0.1127 (2) | 0.6394 (4) | 0.0355 (11) |
| O9 | 0.32412 (19) | 0.1439 (3) | 0.5897 (4) | 0.0333 (11) |
| O10 | 0.3722 (2) | 0.0854 (3) | 0.7370 (4) | 0.0372 (12) |
| O11 | 0.3952 (2) | 0.1009 (3) | 0.9240 (4) | 0.0407 (13) |
| O12 | 0.45956 (19) | 0.2814 (3) | 0.9252 (4) | 0.0349 (11) |
| O13 | 0.3888 (2) | 0.2209 (3) | 1.0310 (4) | 0.0420 (13) |
| O14 | 0.3515 (2) | 0.3523 (3) | 0.9652 (4) | 0.0374 (12) |
| O15 | 0.30057 (19) | 0.4081 (3) | 0.8207 (4) | 0.0337 (11) |
| O16 | 0.1992 (2) | 0.3743 (4) | 0.8289 (5) | 0.0527 (16) |

| | | | | |
|-----|--------------|------------|-------------|-------------|
| O17 | 0.25496 (19) | 0.3787 (3) | 0.6547 (4) | 0.0363 (11) |
| O18 | 0.22650 (19) | 0.2506 (3) | 0.7233 (4) | 0.0377 (12) |
| O19 | 0.32137 (16) | 0.2804 (2) | 0.7018 (3) | 0.0231 (9) |
| O20 | 0.36948 (17) | 0.2233 (2) | 0.8397 (3) | 0.0257 (9) |
| O21 | 0.39628 (16) | 0.3431 (2) | 0.7695 (3) | 0.0241 (8) |
| O22 | 0.40539 (17) | 0.2288 (2) | 0.6696 (3) | 0.0248 (9) |
| O23 | 0.35674 (19) | 0.2989 (3) | 0.5004 (4) | 0.0344 (11) |
| O24 | 0.4401 (3) | 0.2850 (4) | 0.3828 (4) | 0.0512 (15) |
| O25 | 0.43539 (19) | 0.3610 (3) | 0.5671 (4) | 0.0342 (11) |
| O26 | 0.48598 (18) | 0.2386 (3) | 0.5597 (4) | 0.0340 (11) |
| O27 | 0.4063 (2) | 0.1693 (3) | 0.4917 (4) | 0.0349 (11) |
| O28 | 0.3447 (2) | 0.5055 (3) | 0.9514 (5) | 0.0499 (15) |
| O29 | 0.38277 (19) | 0.4838 (2) | 0.7624 (4) | 0.0361 (11) |
| O30 | 0.43123 (19) | 0.4244 (3) | 0.9129 (4) | 0.0344 (11) |
| O31 | 0.3075 (2) | 0.1592 (3) | 0.9607 (4) | 0.0440 (14) |
| O32 | 0.4708 (2) | 0.1659 (3) | 0.8178 (4) | 0.0341 (11) |
| O33 | 0.4791 (3) | 0.1462 (4) | 1.0216 (5) | 0.0547 (16) |
| O34 | 0.2843 (2) | 0.1389 (3) | 0.7637 (4) | 0.0367 (11) |
| O35 | 0.4338 (2) | 0.5098 (3) | 0.5822 (5) | 0.0488 (15) |
| O36 | 0.2790 (2) | 0.3974 (3) | 0.4560 (4) | 0.0446 (14) |
| N1 | 0.6761 (3) | 0.4097 (4) | 0.0486 (6) | 0.0457 (17) |
| N2 | 0.5963 (3) | 0.3569 (4) | 0.5746 (5) | 0.0438 (16) |
| N3 | 0.7647 (3) | 0.3614 (4) | 0.3484 (6) | 0.0437 (16) |
| N4 | 0.5971 (3) | 0.1673 (3) | -0.0459 (5) | 0.0390 (15) |
| N5 | 0.4821 (3) | 0.3901 (4) | 0.2356 (6) | 0.0476 (18) |
| O47 | 0.6329 (3) | 0.1665 (4) | 0.4103 (5) | 0.0617 (19) |
| N7 | 0.6224 (3) | 0.0801 (4) | 0.5252 (5) | 0.0400 (15) |
| N8 | 0.4832 (3) | 0.1029 (4) | 0.2582 (6) | 0.0474 (17) |
| N9 | 0.7415 (3) | 0.0838 (4) | 0.1778 (6) | 0.0471 (17) |
| O37 | 0.2743 (2) | 0.2842 (3) | 0.8971 (4) | 0.0382 (12) |
| O38 | 0.2989 (3) | 0.2710 (4) | 1.1019 (4) | 0.0632 (19) |
| O39 | 0.3086 (3) | 0.0201 (3) | 0.8810 (5) | 0.0559 (17) |
| O55 | 0.5523 (2) | 0.1732 (3) | 0.6856 (5) | 0.0459 (14) |
| O40 | 0.6550 (2) | 0.3481 (3) | 0.1859 (5) | 0.0490 (14) |
| C2 | 0.6452 (3) | 0.3714 (4) | 0.1012 (7) | 0.046 (2) |
| H8 | 0.6142 | 0.3609 | 0.0743 | 0.055* |
| C3 | 0.7237 (4) | 0.4299 (5) | 0.0907 (9) | 0.061 (3) |
| H2 | 0.7185 | 0.4556 | 0.1520 | 0.092* |
| H3 | 0.7412 | 0.4606 | 0.0448 | 0.092* |
| H4 | 0.7429 | 0.3867 | 0.1032 | 0.092* |
| C4 | 0.6638 (5) | 0.4329 (6) | -0.0517 (7) | 0.067 (3) |
| H6 | 0.6861 | 0.4101 | -0.0980 | 0.101* |
| H7 | 0.6670 | 0.4849 | -0.0564 | 0.101* |
| H5 | 0.6303 | 0.4191 | -0.0668 | 0.101* |
| O41 | 0.6001 (3) | 0.3175 (4) | 0.4158 (5) | 0.0580 (17) |
| C6 | 0.6147 (3) | 0.3158 (5) | 0.5037 (7) | 0.051 (2) |
| H10 | 0.6400 | 0.2836 | 0.5200 | 0.062* |
| C7 | 0.6139 (4) | 0.3522 (7) | 0.6749 (7) | 0.067 (3) |

| | | | | |
|-----|------------|------------|-------------|-------------|
| H12 | 0.6340 | 0.3092 | 0.6823 | 0.100* |
| H13 | 0.5861 | 0.3496 | 0.7195 | 0.100* |
| H11 | 0.6335 | 0.3945 | 0.6902 | 0.100* |
| C8 | 0.5581 (4) | 0.4096 (6) | 0.5489 (8) | 0.068 (3) |
| H15 | 0.5724 | 0.4481 | 0.5099 | 0.102* |
| H16 | 0.5441 | 0.4297 | 0.6086 | 0.102* |
| H14 | 0.5324 | 0.3860 | 0.5112 | 0.102* |
| O42 | 0.7020 (2) | 0.2798 (3) | 0.3417 (5) | 0.0472 (14) |
| C10 | 0.7180 (3) | 0.3417 (4) | 0.3558 (6) | 0.0430 (18) |
| H18 | 0.6951 | 0.3774 | 0.3731 | 0.052* |
| C11 | 0.8025 (4) | 0.3079 (6) | 0.3206 (8) | 0.062 (3) |
| H19 | 0.7881 | 0.2600 | 0.3203 | 0.093* |
| H20 | 0.8293 | 0.3093 | 0.3678 | 0.093* |
| H21 | 0.8151 | 0.3190 | 0.2555 | 0.093* |
| C12 | 0.7807 (4) | 0.4351 (6) | 0.3660 (9) | 0.067 (3) |
| H22 | 0.7522 | 0.4657 | 0.3761 | 0.100* |
| H23 | 0.7992 | 0.4523 | 0.3096 | 0.100* |
| H24 | 0.8014 | 0.4365 | 0.4241 | 0.100* |
| O43 | 0.6047 (3) | 0.2262 (3) | 0.0990 (4) | 0.0514 (15) |
| C14 | 0.5960 (3) | 0.1715 (4) | 0.0515 (6) | 0.0422 (18) |
| H26 | 0.5881 | 0.1294 | 0.0866 | 0.051* |
| C15 | 0.5833 (4) | 0.1013 (4) | -0.0986 (6) | 0.046 (2) |
| H28 | 0.5798 | 0.0620 | -0.0519 | 0.069* |
| H29 | 0.6087 | 0.0894 | -0.1461 | 0.069* |
| H27 | 0.5523 | 0.1088 | -0.1325 | 0.069* |
| C16 | 0.6085 (4) | 0.2314 (5) | -0.1036 (7) | 0.055 (2) |
| H31 | 0.5807 | 0.2641 | -0.1021 | 0.082* |
| H30 | 0.6153 | 0.2175 | -0.1710 | 0.082* |
| H32 | 0.6372 | 0.2551 | -0.0759 | 0.082* |
| O44 | 0.5498 (2) | 0.3180 (4) | 0.2319 (5) | 0.0528 (16) |
| C18 | 0.5248 (3) | 0.3674 (4) | 0.2680 (8) | 0.0468 (19) |
| H34 | 0.5377 | 0.3907 | 0.3237 | 0.056* |
| C19 | 0.4532 (4) | 0.4425 (5) | 0.2893 (9) | 0.065 (3) |
| H35 | 0.4220 | 0.4211 | 0.3081 | 0.098* |
| H36 | 0.4472 | 0.4842 | 0.2479 | 0.098* |
| H37 | 0.4709 | 0.4573 | 0.3478 | 0.098* |
| C20 | 0.4613 (6) | 0.3597 (9) | 0.1481 (9) | 0.114 (6) |
| H39 | 0.4498 | 0.3982 | 0.1055 | 0.171* |
| H40 | 0.4338 | 0.3289 | 0.1656 | 0.171* |
| H38 | 0.4861 | 0.3316 | 0.1140 | 0.171* |
| C21 | 0.6486 (4) | 0.1287 (5) | 0.4775 (6) | 0.0453 (19) |
| H47 | 0.6816 | 0.1349 | 0.4962 | 0.054* |
| C22 | 0.5722 (3) | 0.0645 (5) | 0.4960 (9) | 0.058 (2) |
| H41 | 0.5499 | 0.0791 | 0.5481 | 0.087* |
| H42 | 0.5687 | 0.0132 | 0.4841 | 0.087* |
| H43 | 0.5645 | 0.0909 | 0.4364 | 0.087* |
| C23 | 0.6432 (4) | 0.0379 (6) | 0.6040 (8) | 0.064 (3) |
| H44 | 0.6776 | 0.0503 | 0.6120 | 0.096* |

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|-----|------------|------------|-------------|-------------|
| H46 | 0.6403 | -0.0130 | 0.5884 | 0.096* |
| H45 | 0.6257 | 0.0480 | 0.6646 | 0.096* |
| O45 | 0.5562 (2) | 0.1600 (3) | 0.2673 (5) | 0.0503 (14) |
| C25 | 0.5106 (3) | 0.1617 (4) | 0.2671 (7) | 0.0449 (19) |
| H55 | 0.4948 | 0.2066 | 0.2735 | 0.054* |
| C26 | 0.5044 (5) | 0.0336 (5) | 0.2361 (11) | 0.088 (4) |
| H49 | 0.5385 | 0.0398 | 0.2165 | 0.133* |
| H51 | 0.4862 | 0.0111 | 0.1830 | 0.133* |
| H50 | 0.5029 | 0.0031 | 0.2941 | 0.133* |
| C27 | 0.4286 (4) | 0.1112 (7) | 0.2546 (9) | 0.080 (4) |
| H52 | 0.4201 | 0.1618 | 0.2609 | 0.120* |
| H53 | 0.4139 | 0.0842 | 0.3081 | 0.120* |
| H54 | 0.4164 | 0.0930 | 0.1923 | 0.120* |
| C28 | 0.7155 (4) | 0.1265 (5) | 0.2333 (7) | 0.050 (2) |
| H56 | 0.7275 | 0.1363 | 0.2968 | 0.060* |
| C29 | 0.7248 (4) | 0.0661 (8) | 0.0795 (9) | 0.084 (4) |
| H58 | 0.7093 | 0.1081 | 0.0501 | 0.126* |
| H59 | 0.7012 | 0.0270 | 0.0829 | 0.126* |
| H57 | 0.7526 | 0.0514 | 0.0396 | 0.126* |
| C30 | 0.7896 (5) | 0.0544 (8) | 0.2084 (9) | 0.088 (4) |
| H61 | 0.8144 | 0.0676 | 0.1603 | 0.132* |
| H62 | 0.7875 | 0.0023 | 0.2129 | 0.132* |
| H60 | 0.7985 | 0.0741 | 0.2721 | 0.132* |
| O52 | 0.3886 (3) | 0.0253 (3) | 0.5521 (5) | 0.0571 (17) |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|------|--------------|--------------|--------------|---------------|---------------|---------------|
| Eu1 | 0.03342 (16) | 0.02974 (14) | 0.03036 (15) | -0.00241 (13) | -0.00034 (15) | -0.00084 (15) |
| Mo1 | 0.0306 (3) | 0.0302 (3) | 0.0392 (3) | -0.0058 (2) | -0.0060 (3) | -0.0007 (3) |
| Mo2 | 0.0306 (3) | 0.0352 (3) | 0.0352 (3) | 0.0008 (2) | -0.0079 (3) | 0.0104 (3) |
| Mo3 | 0.0381 (3) | 0.0250 (3) | 0.0385 (3) | -0.0063 (2) | -0.0028 (3) | 0.0059 (3) |
| Mo4 | 0.0258 (3) | 0.0310 (3) | 0.0333 (3) | 0.0000 (2) | -0.0034 (2) | -0.0058 (3) |
| Mo5 | 0.0281 (3) | 0.0369 (3) | 0.0347 (3) | 0.0098 (2) | -0.0026 (3) | -0.0085 (3) |
| Mo6 | 0.0397 (3) | 0.0252 (3) | 0.0403 (3) | 0.0005 (2) | 0.0023 (3) | -0.0095 (3) |
| Mo7 | 0.0455 (4) | 0.0297 (3) | 0.0399 (4) | -0.0055 (3) | 0.0003 (3) | 0.0121 (3) |
| Mo8 | 0.0409 (4) | 0.0384 (3) | 0.0306 (3) | 0.0043 (3) | -0.0081 (3) | 0.0091 (3) |
| Mo9 | 0.0560 (4) | 0.0450 (4) | 0.0268 (3) | 0.0115 (3) | 0.0128 (3) | 0.0052 (3) |
| Mo10 | 0.0317 (3) | 0.0291 (3) | 0.0447 (4) | 0.0035 (2) | 0.0021 (3) | -0.0131 (3) |
| Mo11 | 0.0238 (3) | 0.0406 (3) | 0.0419 (4) | 0.0031 (2) | 0.0032 (3) | -0.0048 (3) |
| Mo12 | 0.0406 (3) | 0.0386 (3) | 0.0238 (3) | 0.0044 (3) | 0.0064 (3) | 0.0030 (3) |
| P1 | 0.0222 (7) | 0.0199 (6) | 0.0198 (7) | 0.0017 (5) | -0.0004 (5) | 0.0009 (5) |
| O1 | 0.050 (4) | 0.057 (4) | 0.051 (4) | 0.014 (3) | -0.006 (3) | -0.014 (3) |
| O2 | 0.040 (3) | 0.040 (3) | 0.056 (4) | -0.009 (2) | -0.007 (3) | -0.006 (3) |
| O3 | 0.034 (3) | 0.036 (3) | 0.035 (3) | 0.000 (2) | -0.009 (2) | 0.001 (2) |
| O4 | 0.034 (3) | 0.027 (2) | 0.035 (3) | 0.0005 (19) | -0.003 (2) | 0.005 (2) |
| O5 | 0.032 (3) | 0.029 (2) | 0.037 (3) | -0.0049 (19) | 0.000 (2) | -0.002 (2) |
| O6 | 0.031 (3) | 0.043 (3) | 0.052 (3) | -0.004 (2) | -0.013 (2) | -0.009 (3) |

| | | | | | | |
|-----|-----------|-------------|-----------|-------------|--------------|--------------|
| O7 | 0.030 (3) | 0.032 (2) | 0.037 (3) | 0.0019 (19) | 0.002 (2) | -0.004 (2) |
| O8 | 0.038 (3) | 0.027 (2) | 0.042 (3) | 0.008 (2) | 0.002 (2) | -0.007 (2) |
| O9 | 0.035 (3) | 0.031 (2) | 0.033 (3) | 0.001 (2) | -0.005 (2) | -0.006 (2) |
| O10 | 0.044 (3) | 0.029 (2) | 0.039 (3) | 0.004 (2) | 0.000 (2) | 0.001 (2) |
| O11 | 0.051 (3) | 0.032 (3) | 0.040 (3) | 0.004 (2) | -0.005 (3) | 0.009 (2) |
| O12 | 0.037 (3) | 0.035 (3) | 0.032 (3) | 0.004 (2) | 0.001 (2) | 0.000 (2) |
| O13 | 0.054 (3) | 0.051 (3) | 0.021 (2) | 0.007 (3) | -0.003 (2) | 0.004 (2) |
| O14 | 0.043 (3) | 0.040 (3) | 0.030 (3) | 0.006 (2) | 0.002 (2) | -0.003 (2) |
| O15 | 0.029 (3) | 0.032 (2) | 0.040 (3) | 0.003 (2) | 0.002 (2) | -0.003 (2) |
| O16 | 0.032 (3) | 0.061 (4) | 0.065 (4) | 0.007 (3) | 0.011 (3) | -0.009 (3) |
| O17 | 0.031 (3) | 0.034 (2) | 0.044 (3) | 0.007 (2) | -0.002 (2) | 0.005 (2) |
| O18 | 0.026 (3) | 0.040 (3) | 0.047 (3) | -0.004 (2) | 0.003 (2) | 0.000 (2) |
| O19 | 0.025 (2) | 0.0205 (19) | 0.024 (2) | 0.0017 (16) | -0.0012 (17) | 0.0037 (17) |
| O20 | 0.031 (2) | 0.023 (2) | 0.023 (2) | 0.0016 (17) | 0.0007 (18) | 0.0042 (18) |
| O21 | 0.027 (2) | 0.0232 (18) | 0.022 (2) | 0.0028 (16) | 0.0001 (19) | -0.0043 (18) |
| O22 | 0.030 (2) | 0.0222 (19) | 0.022 (2) | 0.0018 (17) | -0.0004 (18) | -0.0021 (17) |
| O23 | 0.035 (3) | 0.038 (3) | 0.031 (3) | 0.002 (2) | -0.003 (2) | -0.001 (2) |
| O24 | 0.064 (4) | 0.061 (4) | 0.028 (3) | 0.005 (3) | 0.016 (3) | 0.006 (3) |
| O25 | 0.032 (3) | 0.035 (2) | 0.036 (3) | -0.001 (2) | 0.000 (2) | -0.003 (2) |
| O26 | 0.029 (2) | 0.039 (3) | 0.033 (3) | 0.006 (2) | 0.007 (2) | -0.004 (2) |
| O27 | 0.042 (3) | 0.038 (3) | 0.025 (2) | 0.006 (2) | -0.002 (2) | -0.008 (2) |
| O28 | 0.050 (4) | 0.038 (3) | 0.062 (4) | 0.006 (3) | 0.004 (3) | -0.024 (3) |
| O29 | 0.038 (3) | 0.0220 (19) | 0.048 (3) | 0.0043 (19) | -0.001 (2) | -0.002 (2) |
| O30 | 0.032 (3) | 0.035 (2) | 0.036 (3) | 0.005 (2) | -0.003 (2) | -0.013 (2) |
| O31 | 0.051 (4) | 0.039 (3) | 0.042 (3) | -0.002 (2) | 0.014 (3) | 0.013 (2) |
| O32 | 0.042 (3) | 0.030 (2) | 0.030 (2) | 0.011 (2) | -0.002 (2) | 0.001 (2) |
| O33 | 0.060 (4) | 0.061 (4) | 0.043 (3) | 0.013 (3) | -0.018 (3) | 0.010 (3) |
| O34 | 0.041 (3) | 0.029 (2) | 0.039 (3) | -0.005 (2) | 0.005 (2) | 0.006 (2) |
| O35 | 0.054 (4) | 0.038 (3) | 0.055 (4) | -0.012 (3) | -0.002 (3) | 0.014 (3) |
| O36 | 0.047 (3) | 0.047 (3) | 0.040 (3) | 0.001 (3) | -0.016 (3) | 0.015 (3) |
| N1 | 0.060 (5) | 0.033 (3) | 0.044 (4) | -0.002 (3) | 0.008 (4) | 0.000 (3) |
| N2 | 0.040 (4) | 0.056 (4) | 0.035 (3) | 0.000 (3) | 0.004 (3) | -0.007 (3) |
| N3 | 0.040 (4) | 0.041 (3) | 0.050 (4) | -0.002 (3) | -0.010 (3) | -0.007 (3) |
| N4 | 0.041 (4) | 0.034 (3) | 0.043 (4) | 0.005 (3) | -0.008 (3) | -0.001 (3) |
| N5 | 0.049 (4) | 0.039 (3) | 0.054 (4) | 0.007 (3) | 0.000 (3) | 0.012 (3) |
| O47 | 0.072 (5) | 0.053 (4) | 0.060 (4) | -0.010 (3) | -0.008 (4) | 0.023 (3) |
| N7 | 0.043 (4) | 0.037 (3) | 0.040 (4) | -0.005 (3) | 0.004 (3) | -0.002 (3) |
| N8 | 0.045 (4) | 0.047 (4) | 0.050 (4) | -0.016 (3) | 0.006 (3) | -0.013 (3) |
| N9 | 0.052 (4) | 0.043 (4) | 0.047 (4) | 0.005 (3) | 0.002 (3) | 0.001 (3) |
| O37 | 0.040 (3) | 0.038 (3) | 0.036 (3) | 0.003 (2) | 0.011 (2) | 0.003 (2) |
| O38 | 0.075 (5) | 0.085 (5) | 0.030 (3) | 0.017 (4) | 0.026 (3) | 0.003 (3) |
| O39 | 0.072 (4) | 0.034 (3) | 0.061 (4) | -0.017 (3) | -0.003 (3) | 0.017 (3) |
| O55 | 0.036 (3) | 0.054 (3) | 0.048 (3) | 0.017 (3) | -0.003 (3) | -0.015 (3) |
| O40 | 0.059 (4) | 0.041 (3) | 0.047 (3) | -0.016 (3) | -0.004 (3) | 0.011 (3) |
| C2 | 0.049 (5) | 0.029 (3) | 0.060 (6) | -0.006 (3) | -0.002 (4) | -0.003 (4) |
| C3 | 0.051 (6) | 0.053 (5) | 0.079 (7) | -0.004 (4) | 0.017 (5) | 0.007 (5) |
| C4 | 0.105 (9) | 0.059 (6) | 0.037 (5) | -0.012 (6) | 0.002 (5) | 0.008 (5) |
| O41 | 0.057 (4) | 0.077 (4) | 0.040 (3) | 0.019 (4) | -0.004 (3) | -0.016 (3) |

| | | | | | | |
|-----|------------|------------|------------|------------|------------|------------|
| C6 | 0.050 (5) | 0.058 (5) | 0.046 (5) | 0.014 (4) | -0.006 (4) | -0.009 (4) |
| C7 | 0.062 (7) | 0.103 (9) | 0.036 (5) | -0.012 (6) | 0.012 (5) | -0.015 (5) |
| C8 | 0.067 (7) | 0.080 (7) | 0.056 (6) | 0.019 (6) | 0.018 (5) | -0.007 (6) |
| O42 | 0.041 (3) | 0.045 (3) | 0.056 (4) | -0.006 (3) | -0.012 (3) | -0.001 (3) |
| C10 | 0.040 (4) | 0.042 (4) | 0.046 (5) | 0.000 (3) | -0.003 (4) | -0.005 (4) |
| C11 | 0.047 (6) | 0.074 (7) | 0.066 (6) | 0.006 (5) | -0.002 (5) | -0.018 (5) |
| C12 | 0.057 (6) | 0.065 (6) | 0.078 (7) | -0.023 (5) | -0.004 (6) | -0.009 (6) |
| O43 | 0.073 (4) | 0.047 (3) | 0.033 (3) | 0.003 (3) | -0.010 (3) | -0.007 (3) |
| C14 | 0.053 (5) | 0.039 (4) | 0.034 (4) | 0.003 (4) | -0.010 (4) | 0.000 (4) |
| C15 | 0.061 (6) | 0.040 (4) | 0.038 (4) | 0.011 (4) | -0.013 (4) | -0.003 (3) |
| C16 | 0.078 (7) | 0.042 (4) | 0.045 (5) | 0.005 (5) | -0.003 (5) | 0.004 (4) |
| O44 | 0.052 (4) | 0.058 (4) | 0.049 (4) | 0.019 (3) | -0.002 (3) | 0.000 (3) |
| C18 | 0.045 (5) | 0.042 (4) | 0.053 (5) | -0.003 (3) | -0.008 (4) | 0.000 (4) |
| C19 | 0.058 (6) | 0.044 (5) | 0.093 (8) | 0.007 (4) | 0.007 (6) | 0.016 (5) |
| C20 | 0.128 (13) | 0.149 (14) | 0.064 (8) | 0.055 (11) | -0.058 (9) | -0.021 (9) |
| C21 | 0.049 (5) | 0.045 (4) | 0.042 (5) | -0.010 (4) | 0.001 (4) | 0.007 (4) |
| C22 | 0.050 (5) | 0.044 (5) | 0.081 (7) | -0.011 (4) | 0.005 (5) | -0.006 (5) |
| C23 | 0.075 (7) | 0.065 (6) | 0.051 (6) | -0.018 (5) | -0.011 (5) | 0.023 (5) |
| O45 | 0.041 (3) | 0.046 (3) | 0.064 (4) | -0.013 (3) | -0.001 (3) | 0.008 (3) |
| C25 | 0.050 (5) | 0.039 (4) | 0.046 (5) | -0.014 (3) | 0.003 (4) | -0.007 (4) |
| C26 | 0.084 (9) | 0.041 (5) | 0.140 (13) | -0.009 (6) | 0.007 (8) | -0.008 (6) |
| C27 | 0.052 (6) | 0.106 (9) | 0.083 (9) | -0.023 (6) | 0.014 (6) | -0.027 (7) |
| C28 | 0.065 (6) | 0.044 (4) | 0.042 (5) | 0.009 (4) | 0.001 (4) | -0.013 (4) |
| C29 | 0.070 (8) | 0.119 (10) | 0.063 (7) | 0.003 (7) | 0.001 (6) | -0.047 (7) |
| C30 | 0.095 (10) | 0.100 (9) | 0.069 (8) | 0.057 (8) | -0.008 (7) | -0.006 (7) |
| O52 | 0.069 (4) | 0.035 (3) | 0.067 (4) | -0.004 (3) | 0.007 (4) | -0.025 (3) |

Geometric parameters (Å, °)

| | | | |
|---------|-----------|---------|------------|
| Eu1—O40 | 2.369 (5) | N1—C3 | 1.450 (12) |
| Eu1—O47 | 2.378 (6) | N1—C4 | 1.452 (12) |
| Eu1—O1 | 2.383 (6) | N2—C6 | 1.311 (11) |
| Eu1—O45 | 2.387 (5) | N2—C7 | 1.433 (12) |
| Eu1—O41 | 2.395 (6) | N2—C8 | 1.455 (12) |
| Eu1—O44 | 2.413 (6) | N3—C10 | 1.312 (11) |
| Eu1—O42 | 2.415 (6) | N3—C12 | 1.438 (11) |
| Eu1—O43 | 2.416 (6) | N3—C11 | 1.463 (12) |
| Mo1—O2 | 1.672 (5) | N4—C14 | 1.313 (10) |
| Mo1—O9 | 1.836 (5) | N4—C16 | 1.441 (11) |
| Mo1—O3 | 1.852 (5) | N4—C15 | 1.452 (10) |
| Mo1—O34 | 1.973 (5) | N5—C18 | 1.297 (11) |
| Mo1—O18 | 1.986 (5) | N5—C20 | 1.417 (14) |
| Mo1—O19 | 2.436 (4) | N5—C19 | 1.433 (12) |
| Mo2—O36 | 1.690 (5) | O47—C21 | 1.214 (11) |
| Mo2—O4 | 1.831 (5) | N7—C21 | 1.307 (10) |
| Mo2—O17 | 1.866 (5) | N7—C23 | 1.427 (12) |
| Mo2—O23 | 1.957 (5) | N7—C22 | 1.435 (11) |
| Mo2—O3 | 1.993 (5) | N8—C25 | 1.313 (10) |

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|----------|-----------|---------|------------|
| Mo2—O19 | 2.429 (4) | N8—C26 | 1.427 (13) |
| Mo3—O35 | 1.672 (5) | N8—C27 | 1.477 (13) |
| Mo3—O25 | 1.842 (5) | N9—C28 | 1.290 (11) |
| Mo3—O5 | 1.848 (5) | N9—C29 | 1.435 (13) |
| Mo3—O4 | 1.985 (5) | N9—C30 | 1.461 (14) |
| Mo3—O29 | 1.985 (5) | O40—C2 | 1.245 (11) |
| Mo3—O21 | 2.428 (4) | C2—H8 | 0.9300 |
| Mo4—O6 | 1.677 (5) | C3—H2 | 0.9600 |
| Mo4—O12 | 1.834 (5) | C3—H3 | 0.9600 |
| Mo4—O30 | 1.851 (5) | C3—H4 | 0.9600 |
| Mo4—O5 | 1.976 (5) | C4—H6 | 0.9600 |
| Mo4—O7 | 1.992 (5) | C4—H7 | 0.9600 |
| Mo4—O21 | 2.426 (4) | C4—H5 | 0.9600 |
| Mo5—O55 | 1.675 (5) | O41—C6 | 1.245 (11) |
| Mo5—O7 | 1.825 (5) | C6—H10 | 0.9300 |
| Mo5—O26 | 1.845 (5) | C7—H12 | 0.9600 |
| Mo5—O32 | 1.979 (5) | C7—H13 | 0.9600 |
| Mo5—O8 | 1.985 (5) | C7—H11 | 0.9600 |
| Mo5—O22 | 2.428 (5) | C8—H15 | 0.9600 |
| Mo6—O52 | 1.676 (5) | C8—H16 | 0.9600 |
| Mo6—O10 | 1.837 (5) | C8—H14 | 0.9600 |
| Mo6—O8 | 1.852 (5) | O42—C10 | 1.228 (9) |
| Mo6—O9 | 1.983 (5) | C10—H18 | 0.9300 |
| Mo6—O27 | 2.000 (5) | C11—H19 | 0.9600 |
| Mo6—O22 | 2.416 (4) | C11—H20 | 0.9600 |
| Mo7—O39 | 1.686 (5) | C11—H21 | 0.9600 |
| Mo7—O34 | 1.842 (6) | C12—H22 | 0.9600 |
| Mo7—O31 | 1.854 (6) | C12—H23 | 0.9600 |
| Mo7—O10 | 1.973 (6) | C12—H24 | 0.9600 |
| Mo7—O11 | 1.994 (6) | O43—C14 | 1.214 (10) |
| Mo7—O20 | 2.438 (4) | C14—H26 | 0.9300 |
| Mo8—O33 | 1.675 (6) | C15—H28 | 0.9600 |
| Mo8—O11 | 1.844 (6) | C15—H29 | 0.9600 |
| Mo8—O32 | 1.853 (5) | C15—H27 | 0.9600 |
| Mo8—O12 | 1.983 (5) | C16—H31 | 0.9600 |
| Mo8—O13 | 1.987 (6) | C16—H30 | 0.9600 |
| Mo8—O20 | 2.423 (4) | C16—H32 | 0.9600 |
| Mo9—O38 | 1.680 (6) | O44—C18 | 1.229 (10) |
| Mo9—O14 | 1.838 (6) | C18—H34 | 0.9300 |
| Mo9—O13 | 1.851 (6) | C19—H35 | 0.9600 |
| Mo9—O31 | 1.984 (6) | C19—H36 | 0.9600 |
| Mo9—O37 | 1.993 (6) | C19—H37 | 0.9600 |
| Mo9—O20 | 2.433 (5) | C20—H39 | 0.9600 |
| Mo10—O28 | 1.690 (5) | C20—H40 | 0.9600 |
| Mo10—O15 | 1.842 (5) | C20—H38 | 0.9600 |
| Mo10—O29 | 1.847 (6) | C21—H47 | 0.9300 |
| Mo10—O14 | 1.976 (5) | C22—H41 | 0.9600 |
| Mo10—O30 | 1.984 (5) | C22—H42 | 0.9600 |

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|-------------|------------|---------------|------------|
| Mo10—O21 | 2.420 (4) | C22—H43 | 0.9600 |
| Mo11—O16 | 1.676 (6) | C23—H44 | 0.9600 |
| Mo11—O37 | 1.836 (5) | C23—H46 | 0.9600 |
| Mo11—O18 | 1.857 (5) | C23—H45 | 0.9600 |
| Mo11—O15 | 1.976 (5) | O45—C25 | 1.227 (10) |
| Mo11—O17 | 1.979 (5) | C25—H55 | 0.9300 |
| Mo11—O19 | 2.423 (4) | C26—H49 | 0.9600 |
| Mo12—O24 | 1.684 (5) | C26—H51 | 0.9600 |
| Mo12—O23 | 1.840 (5) | C26—H50 | 0.9600 |
| Mo12—O27 | 1.850 (5) | C27—H52 | 0.9600 |
| Mo12—O25 | 1.976 (5) | C27—H53 | 0.9600 |
| Mo12—O26 | 1.980 (5) | C27—H54 | 0.9600 |
| Mo12—O22 | 2.428 (4) | C28—H56 | 0.9300 |
| P1—O19 | 1.521 (5) | C29—H58 | 0.9600 |
| P1—O20 | 1.526 (5) | C29—H59 | 0.9600 |
| P1—O22 | 1.527 (5) | C29—H57 | 0.9600 |
| P1—O21 | 1.536 (4) | C30—H61 | 0.9600 |
| O1—C28 | 1.219 (11) | C30—H62 | 0.9600 |
| N1—C2 | 1.297 (11) | C30—H60 | 0.9600 |
| | | | |
| O40—Eu1—O47 | 145.6 (2) | O26—Mo12—O22 | 72.45 (18) |
| O40—Eu1—O1 | 98.6 (2) | O19—P1—O20 | 109.8 (3) |
| O47—Eu1—O1 | 76.7 (2) | O19—P1—O22 | 109.5 (3) |
| O40—Eu1—O45 | 141.7 (2) | O20—P1—O22 | 109.1 (2) |
| O47—Eu1—O45 | 72.7 (2) | O19—P1—O21 | 109.3 (2) |
| O1—Eu1—O45 | 88.5 (2) | O20—P1—O21 | 109.5 (3) |
| O40—Eu1—O41 | 93.6 (2) | O22—P1—O21 | 109.6 (3) |
| O47—Eu1—O41 | 75.1 (3) | C28—O1—Eu1 | 137.4 (6) |
| O1—Eu1—O41 | 145.4 (2) | Mo1—O3—Mo2 | 124.5 (3) |
| O45—Eu1—O41 | 101.7 (2) | Mo2—O4—Mo3 | 151.4 (3) |
| O40—Eu1—O44 | 76.2 (2) | Mo3—O5—Mo4 | 125.8 (3) |
| O47—Eu1—O44 | 127.6 (2) | Mo5—O7—Mo4 | 151.7 (3) |
| O1—Eu1—O44 | 142.6 (2) | Mo6—O8—Mo5 | 124.8 (2) |
| O45—Eu1—O44 | 75.6 (2) | Mo1—O9—Mo6 | 151.6 (3) |
| O41—Eu1—O44 | 71.8 (2) | Mo6—O10—Mo7 | 151.5 (3) |
| O40—Eu1—O42 | 70.2 (2) | Mo8—O11—Mo7 | 125.5 (3) |
| O47—Eu1—O42 | 75.6 (2) | Mo4—O12—Mo8 | 152.1 (3) |
| O1—Eu1—O42 | 76.8 (2) | Mo9—O13—Mo8 | 124.6 (3) |
| O45—Eu1—O42 | 147.4 (2) | Mo9—O14—Mo10 | 151.8 (3) |
| O41—Eu1—O42 | 77.2 (2) | Mo10—O15—Mo11 | 151.4 (3) |
| O44—Eu1—O42 | 132.0 (2) | Mo2—O17—Mo11 | 124.8 (3) |
| O40—Eu1—O43 | 73.5 (2) | Mo11—O18—Mo1 | 124.6 (3) |
| O47—Eu1—O43 | 132.8 (2) | P1—O19—Mo11 | 126.2 (2) |
| O1—Eu1—O43 | 70.2 (2) | P1—O19—Mo2 | 125.7 (2) |
| O45—Eu1—O43 | 73.7 (2) | Mo11—O19—Mo2 | 89.23 (14) |
| O41—Eu1—O43 | 144.3 (2) | P1—O19—Mo1 | 126.1 (2) |
| O44—Eu1—O43 | 72.8 (2) | Mo11—O19—Mo1 | 88.93 (15) |
| O42—Eu1—O43 | 125.7 (2) | Mo2—O19—Mo1 | 88.80 (15) |

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| O2—Mo1—O9 | 102.7 (3) | P1—O20—Mo8 | 126.5 (3) |
| O2—Mo1—O3 | 102.4 (3) | P1—O20—Mo9 | 125.6 (2) |
| O9—Mo1—O3 | 95.8 (2) | Mo8—O20—Mo9 | 88.87 (15) |
| O2—Mo1—O34 | 101.0 (3) | P1—O20—Mo7 | 125.7 (3) |
| O9—Mo1—O34 | 85.0 (2) | Mo8—O20—Mo7 | 89.20 (14) |
| O3—Mo1—O34 | 155.8 (2) | Mo9—O20—Mo7 | 89.09 (15) |
| O2—Mo1—O18 | 100.5 (3) | P1—O21—Mo10 | 126.1 (3) |
| O9—Mo1—O18 | 155.7 (2) | P1—O21—Mo4 | 125.6 (2) |
| O3—Mo1—O18 | 86.5 (2) | Mo10—O21—Mo4 | 89.12 (14) |
| O34—Mo1—O18 | 83.2 (2) | P1—O21—Mo3 | 126.0 (3) |
| O2—Mo1—O19 | 171.9 (2) | Mo10—O21—Mo3 | 89.13 (13) |
| O9—Mo1—O19 | 85.20 (18) | Mo4—O21—Mo3 | 89.11 (14) |
| O3—Mo1—O19 | 74.36 (18) | P1—O22—Mo6 | 126.0 (3) |
| O34—Mo1—O19 | 81.65 (18) | P1—O22—Mo5 | 126.1 (3) |
| O18—Mo1—O19 | 72.08 (18) | Mo6—O22—Mo5 | 89.19 (14) |
| O36—Mo2—O4 | 103.7 (2) | P1—O22—Mo12 | 126.0 (2) |
| O36—Mo2—O17 | 102.2 (3) | Mo6—O22—Mo12 | 89.10 (14) |
| O4—Mo2—O17 | 95.3 (2) | Mo5—O22—Mo12 | 88.42 (15) |
| O36—Mo2—O23 | 101.5 (3) | Mo12—O23—Mo2 | 152.1 (3) |
| O4—Mo2—O23 | 85.7 (2) | Mo3—O25—Mo12 | 152.5 (3) |
| O17—Mo2—O23 | 155.4 (2) | Mo5—O26—Mo12 | 124.5 (3) |
| O36—Mo2—O3 | 98.6 (3) | Mo12—O27—Mo6 | 123.9 (3) |
| O4—Mo2—O3 | 156.8 (2) | Mo10—O29—Mo3 | 125.1 (2) |
| O17—Mo2—O3 | 86.4 (2) | Mo4—O30—Mo10 | 124.8 (3) |
| O23—Mo2—O3 | 83.5 (2) | Mo7—O31—Mo9 | 125.8 (3) |
| O36—Mo2—O19 | 170.1 (2) | Mo8—O32—Mo5 | 151.7 (3) |
| O4—Mo2—O19 | 85.87 (18) | Mo7—O34—Mo1 | 152.0 (3) |
| O17—Mo2—O19 | 73.79 (19) | C2—N1—C3 | 119.4 (8) |
| O23—Mo2—O19 | 81.74 (18) | C2—N1—C4 | 121.4 (9) |
| O3—Mo2—O19 | 72.30 (18) | C3—N1—C4 | 119.2 (8) |
| O35—Mo3—O25 | 102.3 (3) | C6—N2—C7 | 121.7 (8) |
| O35—Mo3—O5 | 102.5 (3) | C6—N2—C8 | 118.4 (8) |
| O25—Mo3—O5 | 96.1 (2) | C7—N2—C8 | 119.9 (8) |
| O35—Mo3—O4 | 102.0 (3) | C10—N3—C12 | 122.2 (8) |
| O25—Mo3—O4 | 84.4 (2) | C10—N3—C11 | 120.0 (7) |
| O5—Mo3—O4 | 154.8 (2) | C12—N3—C11 | 117.8 (8) |
| O35—Mo3—O29 | 100.9 (3) | C14—N4—C16 | 119.6 (7) |
| O25—Mo3—O29 | 155.3 (2) | C14—N4—C15 | 122.0 (7) |
| O5—Mo3—O29 | 87.0 (2) | C16—N4—C15 | 118.2 (7) |
| O4—Mo3—O29 | 82.7 (2) | C18—N5—C20 | 120.2 (9) |
| O35—Mo3—O21 | 171.5 (2) | C18—N5—C19 | 121.8 (9) |
| O25—Mo3—O21 | 85.71 (19) | C20—N5—C19 | 117.9 (10) |
| O5—Mo3—O21 | 73.44 (19) | C21—O47—Eu1 | 166.5 (7) |
| O4—Mo3—O21 | 81.45 (17) | C21—N7—C23 | 121.6 (8) |
| O29—Mo3—O21 | 71.66 (17) | C21—N7—C22 | 120.6 (8) |
| O6—Mo4—O12 | 103.5 (3) | C23—N7—C22 | 117.7 (8) |
| O6—Mo4—O30 | 103.7 (2) | C25—N8—C26 | 121.7 (9) |
| O12—Mo4—O30 | 96.0 (2) | C25—N8—C27 | 118.5 (9) |

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| O6—Mo4—O5 | 99.6 (2) | C26—N8—C27 | 118.9 (9) |
| O12—Mo4—O5 | 155.3 (2) | C28—N9—C29 | 120.0 (9) |
| O30—Mo4—O5 | 87.0 (2) | C28—N9—C30 | 122.9 (9) |
| O6—Mo4—O7 | 100.0 (2) | C29—N9—C30 | 117.0 (9) |
| O12—Mo4—O7 | 85.3 (2) | Mo11—O37—Mo9 | 151.5 (3) |
| O30—Mo4—O7 | 155.2 (2) | C2—O40—Eu1 | 130.2 (5) |
| O5—Mo4—O7 | 82.0 (2) | O40—C2—N1 | 123.4 (9) |
| O6—Mo4—O21 | 170.8 (2) | O40—C2—H8 | 118.3 |
| O12—Mo4—O21 | 85.6 (2) | N1—C2—H8 | 118.3 |
| O30—Mo4—O21 | 73.97 (19) | N1—C3—H2 | 109.5 |
| O5—Mo4—O21 | 71.54 (18) | N1—C3—H3 | 109.5 |
| O7—Mo4—O21 | 81.47 (18) | H2—C3—H3 | 109.5 |
| O55—Mo5—O7 | 103.4 (3) | N1—C3—H4 | 109.5 |
| O55—Mo5—O26 | 102.0 (3) | H2—C3—H4 | 109.5 |
| O7—Mo5—O26 | 96.1 (2) | H3—C3—H4 | 109.5 |
| O55—Mo5—O32 | 101.0 (3) | N1—C4—H6 | 109.5 |
| O7—Mo5—O32 | 85.1 (2) | N1—C4—H7 | 109.5 |
| O26—Mo5—O32 | 156.0 (2) | H6—C4—H7 | 109.5 |
| O55—Mo5—O8 | 99.6 (3) | N1—C4—H5 | 109.5 |
| O7—Mo5—O8 | 155.5 (2) | H6—C4—H5 | 109.5 |
| O26—Mo5—O8 | 87.2 (2) | H7—C4—H5 | 109.5 |
| O32—Mo5—O8 | 82.3 (2) | C6—O41—Eu1 | 132.0 (6) |
| O55—Mo5—O22 | 170.7 (2) | O41—C6—N2 | 123.9 (9) |
| O7—Mo5—O22 | 85.67 (19) | O41—C6—H10 | 118.1 |
| O26—Mo5—O22 | 74.59 (18) | N2—C6—H10 | 118.1 |
| O32—Mo5—O22 | 81.61 (18) | N2—C7—H12 | 109.5 |
| O8—Mo5—O22 | 71.80 (17) | N2—C7—H13 | 109.5 |
| O52—Mo6—O10 | 103.3 (3) | H12—C7—H13 | 109.5 |
| O52—Mo6—O8 | 102.5 (3) | N2—C7—H11 | 109.5 |
| O10—Mo6—O8 | 95.8 (2) | H12—C7—H11 | 109.5 |
| O52—Mo6—O9 | 100.9 (3) | H13—C7—H11 | 109.5 |
| O10—Mo6—O9 | 85.6 (2) | N2—C8—H15 | 109.5 |
| O8—Mo6—O9 | 155.5 (2) | N2—C8—H16 | 109.5 |
| O52—Mo6—O27 | 99.1 (3) | H15—C8—H16 | 109.5 |
| O10—Mo6—O27 | 156.2 (2) | N2—C8—H14 | 109.5 |
| O8—Mo6—O27 | 87.2 (2) | H15—C8—H14 | 109.5 |
| O9—Mo6—O27 | 82.1 (2) | H16—C8—H14 | 109.5 |
| O52—Mo6—O22 | 170.8 (3) | C10—O42—Eu1 | 127.1 (5) |
| O10—Mo6—O22 | 85.69 (19) | O42—C10—N3 | 125.4 (8) |
| O8—Mo6—O22 | 74.14 (18) | O42—C10—H18 | 117.3 |
| O9—Mo6—O22 | 81.56 (18) | N3—C10—H18 | 117.3 |
| O27—Mo6—O22 | 72.40 (17) | N3—C11—H19 | 109.5 |
| O39—Mo7—O34 | 103.4 (3) | N3—C11—H20 | 109.5 |
| O39—Mo7—O31 | 102.8 (3) | H19—C11—H20 | 109.5 |
| O34—Mo7—O31 | 96.1 (3) | N3—C11—H21 | 109.5 |
| O39—Mo7—O10 | 102.0 (3) | H19—C11—H21 | 109.5 |
| O34—Mo7—O10 | 85.3 (2) | H20—C11—H21 | 109.5 |
| O31—Mo7—O10 | 154.1 (2) | N3—C12—H22 | 109.5 |

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| O39—Mo7—O11 | 99.8 (3) | N3—C12—H23 | 109.5 |
| O34—Mo7—O11 | 155.4 (2) | H22—C12—H23 | 109.5 |
| O31—Mo7—O11 | 86.4 (3) | N3—C12—H24 | 109.5 |
| O10—Mo7—O11 | 82.1 (2) | H22—C12—H24 | 109.5 |
| O39—Mo7—O20 | 170.4 (3) | H23—C12—H24 | 109.5 |
| O34—Mo7—O20 | 85.93 (18) | C14—O43—Eu1 | 132.6 (5) |
| O31—Mo7—O20 | 73.5 (2) | O43—C14—N4 | 124.7 (8) |
| O10—Mo7—O20 | 80.88 (19) | O43—C14—H26 | 117.6 |
| O11—Mo7—O20 | 71.30 (18) | N4—C14—H26 | 117.6 |
| O33—Mo8—O11 | 102.1 (3) | N4—C15—H28 | 109.5 |
| O33—Mo8—O32 | 103.5 (3) | N4—C15—H29 | 109.5 |
| O11—Mo8—O32 | 96.5 (2) | H28—C15—H29 | 109.5 |
| O33—Mo8—O12 | 101.9 (3) | N4—C15—H27 | 109.5 |
| O11—Mo8—O12 | 155.0 (2) | H28—C15—H27 | 109.5 |
| O32—Mo8—O12 | 84.6 (2) | H29—C15—H27 | 109.5 |
| O33—Mo8—O13 | 98.9 (3) | N4—C16—H31 | 109.5 |
| O11—Mo8—O13 | 86.8 (3) | N4—C16—H30 | 109.5 |
| O32—Mo8—O13 | 156.0 (2) | H31—C16—H30 | 109.5 |
| O12—Mo8—O13 | 82.7 (2) | N4—C16—H32 | 109.5 |
| O33—Mo8—O20 | 170.4 (3) | H31—C16—H32 | 109.5 |
| O11—Mo8—O20 | 74.0 (2) | H30—C16—H32 | 109.5 |
| O32—Mo8—O20 | 85.74 (19) | C18—O44—Eu1 | 138.8 (6) |
| O12—Mo8—O20 | 81.23 (18) | O44—C18—N5 | 126.1 (9) |
| O13—Mo8—O20 | 72.31 (19) | O44—C18—H34 | 117.0 |
| O38—Mo9—O14 | 103.1 (3) | N5—C18—H34 | 117.0 |
| O38—Mo9—O13 | 102.6 (3) | N5—C19—H35 | 109.5 |
| O14—Mo9—O13 | 96.7 (3) | N5—C19—H36 | 109.5 |
| O38—Mo9—O31 | 99.6 (3) | H35—C19—H36 | 109.5 |
| O14—Mo9—O31 | 155.6 (2) | N5—C19—H37 | 109.5 |
| O13—Mo9—O31 | 86.9 (3) | H35—C19—H37 | 109.5 |
| O38—Mo9—O37 | 101.1 (3) | H36—C19—H37 | 109.5 |
| O14—Mo9—O37 | 85.0 (2) | N5—C20—H39 | 109.5 |
| O13—Mo9—O37 | 155.1 (2) | N5—C20—H40 | 109.5 |
| O31—Mo9—O37 | 81.9 (2) | H39—C20—H40 | 109.5 |
| O38—Mo9—O20 | 170.6 (3) | N5—C20—H38 | 109.5 |
| O14—Mo9—O20 | 86.07 (19) | H39—C20—H38 | 109.5 |
| O13—Mo9—O20 | 74.19 (19) | H40—C20—H38 | 109.5 |
| O31—Mo9—O20 | 71.60 (19) | O47—C21—N7 | 124.6 (9) |
| O37—Mo9—O20 | 81.18 (18) | O47—C21—H47 | 117.7 |
| O28—Mo10—O15 | 103.4 (3) | N7—C21—H47 | 117.7 |
| O28—Mo10—O29 | 103.0 (3) | N7—C22—H41 | 109.5 |
| O15—Mo10—O29 | 95.3 (2) | N7—C22—H42 | 109.5 |
| O28—Mo10—O14 | 100.5 (3) | H41—C22—H42 | 109.5 |
| O15—Mo10—O14 | 85.4 (2) | N7—C22—H43 | 109.5 |
| O29—Mo10—O14 | 155.7 (2) | H41—C22—H43 | 109.5 |
| O28—Mo10—O30 | 99.6 (3) | H42—C22—H43 | 109.5 |
| O15—Mo10—O30 | 155.7 (2) | N7—C23—H44 | 109.5 |
| O29—Mo10—O30 | 87.1 (2) | N7—C23—H46 | 109.5 |

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| O14—Mo10—O30 | 82.7 (2) | H44—C23—H46 | 109.5 |
| O28—Mo10—O21 | 171.0 (2) | N7—C23—H45 | 109.5 |
| O15—Mo10—O21 | 85.38 (19) | H44—C23—H45 | 109.5 |
| O29—Mo10—O21 | 74.00 (18) | H46—C23—H45 | 109.5 |
| O14—Mo10—O21 | 81.87 (18) | C25—O45—Eu1 | 136.7 (6) |
| O30—Mo10—O21 | 72.04 (17) | O45—C25—N8 | 122.8 (8) |
| O16—Mo11—O37 | 104.0 (3) | O45—C25—H55 | 118.6 |
| O16—Mo11—O18 | 103.5 (3) | N8—C25—H55 | 118.6 |
| O37—Mo11—O18 | 95.7 (2) | N8—C26—H49 | 109.5 |
| O16—Mo11—O15 | 99.8 (3) | N8—C26—H51 | 109.5 |
| O37—Mo11—O15 | 85.6 (2) | H49—C26—H51 | 109.5 |
| O18—Mo11—O15 | 155.6 (2) | N8—C26—H50 | 109.5 |
| O16—Mo11—O17 | 98.8 (3) | H49—C26—H50 | 109.5 |
| O37—Mo11—O17 | 155.7 (2) | H51—C26—H50 | 109.5 |
| O18—Mo11—O17 | 86.8 (2) | N8—C27—H52 | 109.5 |
| O15—Mo11—O17 | 82.4 (2) | N8—C27—H53 | 109.5 |
| O16—Mo11—O19 | 170.7 (3) | H52—C27—H53 | 109.5 |
| O37—Mo11—O19 | 85.24 (19) | N8—C27—H54 | 109.5 |
| O18—Mo11—O19 | 74.38 (19) | H52—C27—H54 | 109.5 |
| O15—Mo11—O19 | 81.50 (18) | H53—C27—H54 | 109.5 |
| O17—Mo11—O19 | 72.16 (18) | O1—C28—N9 | 125.3 (9) |
| O24—Mo12—O23 | 102.9 (3) | O1—C28—H56 | 117.4 |
| O24—Mo12—O27 | 101.4 (3) | N9—C28—H56 | 117.4 |
| O23—Mo12—O27 | 95.4 (2) | N9—C29—H58 | 109.5 |
| O24—Mo12—O25 | 101.9 (3) | N9—C29—H59 | 109.5 |
| O23—Mo12—O25 | 84.4 (2) | H58—C29—H59 | 109.5 |
| O27—Mo12—O25 | 156.2 (2) | N9—C29—H57 | 109.5 |
| O24—Mo12—O26 | 100.0 (3) | H58—C29—H57 | 109.5 |
| O23—Mo12—O26 | 155.8 (2) | H59—C29—H57 | 109.5 |
| O27—Mo12—O26 | 87.7 (2) | N9—C30—H61 | 109.5 |
| O25—Mo12—O26 | 83.2 (2) | N9—C30—H62 | 109.5 |
| O24—Mo12—O22 | 171.3 (3) | H61—C30—H62 | 109.5 |
| O23—Mo12—O22 | 85.27 (19) | N9—C30—H60 | 109.5 |
| O27—Mo12—O22 | 74.48 (18) | H61—C30—H60 | 109.5 |
| O25—Mo12—O22 | 81.80 (18) | H62—C30—H60 | 109.5 |
| O2—Mo1—O3—Mo2 | 171.0 (3) | O22—P1—O21—Mo10 | 175.5 (3) |
| O9—Mo1—O3—Mo2 | -84.6 (3) | O19—P1—O21—Mo4 | 175.3 (3) |
| O34—Mo1—O3—Mo2 | 6.0 (8) | O20—P1—O21—Mo4 | 55.0 (4) |
| O18—Mo1—O3—Mo2 | 71.1 (3) | O22—P1—O21—Mo4 | -64.6 (4) |
| O19—Mo1—O3—Mo2 | -1.3 (3) | O19—P1—O21—Mo3 | -64.9 (3) |
| O36—Mo2—O4—Mo3 | -129.9 (6) | O20—P1—O21—Mo3 | 174.7 (3) |
| O17—Mo2—O4—Mo3 | 126.1 (6) | O22—P1—O21—Mo3 | 55.1 (3) |
| O23—Mo2—O4—Mo3 | -29.1 (6) | O19—P1—O22—Mo6 | -64.7 (3) |
| O3—Mo2—O4—Mo3 | 33.1 (10) | O20—P1—O22—Mo6 | 55.5 (4) |
| O19—Mo2—O4—Mo3 | 52.9 (6) | O21—P1—O22—Mo6 | 175.3 (3) |
| O35—Mo3—O5—Mo4 | 169.8 (3) | O19—P1—O22—Mo5 | 174.7 (3) |
| O25—Mo3—O5—Mo4 | -86.2 (3) | O20—P1—O22—Mo5 | -65.1 (3) |

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| O4—Mo3—O5—Mo4 | 3.4 (7) | O21—P1—O22—Mo5 | 54.8 (4) |
| O29—Mo3—O5—Mo4 | 69.3 (3) | O19—P1—O22—Mo12 | 55.5 (4) |
| O21—Mo3—O5—Mo4 | -2.5 (3) | O20—P1—O22—Mo12 | 175.7 (3) |
| O55—Mo5—O7—Mo4 | -129.4 (6) | O21—P1—O22—Mo12 | -64.4 (4) |
| O26—Mo5—O7—Mo4 | 126.7 (6) | O24—Mo12—O23—Mo2 | -130.2 (6) |
| O32—Mo5—O7—Mo4 | -29.2 (6) | O27—Mo12—O23—Mo2 | 126.8 (6) |
| O8—Mo5—O7—Mo4 | 30.1 (10) | O25—Mo12—O23—Mo2 | -29.3 (6) |
| O22—Mo5—O7—Mo4 | 52.8 (6) | O26—Mo12—O23—Mo2 | 30.3 (10) |
| O52—Mo6—O8—Mo5 | 168.5 (4) | O22—Mo12—O23—Mo2 | 52.9 (6) |
| O10—Mo6—O8—Mo5 | -86.5 (3) | O35—Mo3—O25—Mo12 | -132.4 (7) |
| O9—Mo6—O8—Mo5 | 5.7 (8) | O5—Mo3—O25—Mo12 | 123.3 (7) |
| O27—Mo6—O8—Mo5 | 69.8 (3) | O4—Mo3—O25—Mo12 | -31.3 (6) |
| O22—Mo6—O8—Mo5 | -2.7 (3) | O29—Mo3—O25—Mo12 | 27.3 (10) |
| O2—Mo1—O9—Mo6 | -129.2 (6) | O21—Mo3—O25—Mo12 | 50.5 (6) |
| O3—Mo1—O9—Mo6 | 126.6 (6) | O55—Mo5—O26—Mo12 | 169.1 (3) |
| O34—Mo1—O9—Mo6 | -29.1 (6) | O7—Mo5—O26—Mo12 | -85.8 (3) |
| O18—Mo1—O9—Mo6 | 32.2 (10) | O32—Mo5—O26—Mo12 | 5.8 (7) |
| O19—Mo1—O9—Mo6 | 52.9 (6) | O8—Mo5—O26—Mo12 | 69.8 (3) |
| O52—Mo6—O10—Mo7 | -128.1 (7) | O22—Mo5—O26—Mo12 | -2.0 (3) |
| O8—Mo6—O10—Mo7 | 127.5 (7) | O24—Mo12—O27—Mo6 | 169.1 (3) |
| O9—Mo6—O10—Mo7 | -27.9 (7) | O23—Mo12—O27—Mo6 | -86.6 (3) |
| O27—Mo6—O10—Mo7 | 31.2 (11) | O25—Mo12—O27—Mo6 | 1.8 (8) |
| O22—Mo6—O10—Mo7 | 54.0 (7) | O26—Mo12—O27—Mo6 | 69.4 (3) |
| O33—Mo8—O11—Mo7 | 168.8 (4) | O22—Mo12—O27—Mo6 | -3.0 (3) |
| O32—Mo8—O11—Mo7 | -85.8 (4) | O28—Mo10—O29—Mo3 | 168.8 (3) |
| O12—Mo8—O11—Mo7 | 5.2 (8) | O15—Mo10—O29—Mo3 | -86.1 (3) |
| O13—Mo8—O11—Mo7 | 70.3 (4) | O14—Mo10—O29—Mo3 | 4.4 (8) |
| O20—Mo8—O11—Mo7 | -2.2 (3) | O30—Mo10—O29—Mo3 | 69.6 (3) |
| O6—Mo4—O12—Mo8 | -128.2 (6) | O21—Mo10—O29—Mo3 | -2.5 (3) |
| O30—Mo4—O12—Mo8 | 126.1 (6) | O6—Mo4—O30—Mo10 | 168.6 (3) |
| O5—Mo4—O12—Mo8 | 30.3 (10) | O12—Mo4—O30—Mo10 | -85.9 (4) |
| O7—Mo4—O12—Mo8 | -29.0 (6) | O5—Mo4—O30—Mo10 | 69.4 (3) |
| O21—Mo4—O12—Mo8 | 52.8 (6) | O7—Mo4—O30—Mo10 | 5.8 (8) |
| O38—Mo9—O13—Mo8 | 169.0 (4) | O21—Mo4—O30—Mo10 | -2.2 (3) |
| O14—Mo9—O13—Mo8 | -85.8 (4) | O39—Mo7—O31—Mo9 | 168.4 (4) |
| O31—Mo9—O13—Mo8 | 69.9 (4) | O34—Mo7—O31—Mo9 | -86.3 (4) |
| O37—Mo9—O13—Mo8 | 6.8 (9) | O10—Mo7—O31—Mo9 | 5.5 (8) |
| O20—Mo9—O13—Mo8 | -1.9 (3) | O11—Mo7—O31—Mo9 | 69.2 (4) |
| O38—Mo9—O14—Mo10 | -131.0 (7) | O20—Mo7—O31—Mo9 | -2.4 (3) |
| O13—Mo9—O14—Mo10 | 124.3 (7) | O33—Mo8—O32—Mo5 | -132.1 (7) |
| O31—Mo9—O14—Mo10 | 27.0 (11) | O11—Mo8—O32—Mo5 | 123.8 (7) |
| O37—Mo9—O14—Mo10 | -30.7 (6) | O12—Mo8—O32—Mo5 | -31.1 (7) |
| O20—Mo9—O14—Mo10 | 50.8 (6) | O13—Mo8—O32—Mo5 | 27.1 (11) |
| O28—Mo10—O15—Mo11 | -128.4 (6) | O20—Mo8—O32—Mo5 | 50.5 (6) |
| O29—Mo10—O15—Mo11 | 126.9 (6) | O39—Mo7—O34—Mo1 | -131.2 (6) |
| O14—Mo10—O15—Mo11 | -28.7 (6) | O31—Mo7—O34—Mo1 | 124.0 (6) |
| O30—Mo10—O15—Mo11 | 32.1 (10) | O10—Mo7—O34—Mo1 | -30.0 (6) |
| O21—Mo10—O15—Mo11 | 53.5 (6) | O11—Mo7—O34—Mo1 | 29.3 (10) |

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| O36—Mo2—O17—Mo11 | 168.2 (3) | O20—Mo7—O34—Mo1 | 51.1 (6) |
| O4—Mo2—O17—Mo11 | -86.5 (3) | O16—Mo11—O37—Mo9 | -127.0 (6) |
| O23—Mo2—O17—Mo11 | 4.5 (7) | O18—Mo11—O37—Mo9 | 127.6 (6) |
| O3—Mo2—O17—Mo11 | 70.2 (3) | O15—Mo11—O37—Mo9 | -28.0 (6) |
| O19—Mo2—O17—Mo11 | -2.4 (3) | O17—Mo11—O37—Mo9 | 32.5 (10) |
| O16—Mo11—O18—Mo1 | 168.6 (4) | O19—Mo11—O37—Mo9 | 53.8 (6) |
| O37—Mo11—O18—Mo1 | -85.5 (4) | Eu1—O40—C2—N1 | -154.9 (6) |
| O15—Mo11—O18—Mo1 | 6.6 (8) | C3—N1—C2—O40 | -3.1 (13) |
| O17—Mo11—O18—Mo1 | 70.3 (3) | C4—N1—C2—O40 | 177.2 (8) |
| O19—Mo11—O18—Mo1 | -2.1 (3) | Eu1—O41—C6—N2 | -176.3 (7) |
| O20—P1—O19—Mo11 | 55.7 (3) | C7—N2—C6—O41 | 179.1 (10) |
| O22—P1—O19—Mo11 | 175.5 (3) | C8—N2—C6—O41 | -2.5 (15) |
| O21—P1—O19—Mo11 | -64.4 (3) | Eu1—O42—C10—N3 | -146.6 (7) |
| O20—P1—O19—Mo2 | 175.9 (3) | C12—N3—C10—O42 | 180.0 (9) |
| O22—P1—O19—Mo2 | -64.3 (3) | C11—N3—C10—O42 | 0.5 (14) |
| O21—P1—O19—Mo2 | 55.8 (4) | Eu1—O43—C14—N4 | -165.4 (6) |
| O20—P1—O19—Mo1 | -64.6 (3) | C16—N4—C14—O43 | -0.9 (14) |
| O22—P1—O19—Mo1 | 55.2 (3) | C15—N4—C14—O43 | -176.1 (8) |
| O21—P1—O19—Mo1 | 175.3 (3) | Eu1—O44—C18—N5 | -169.7 (7) |
| O19—P1—O20—Mo8 | 175.4 (3) | C20—N5—C18—O44 | -3.2 (16) |
| O22—P1—O20—Mo8 | 55.4 (4) | C19—N5—C18—O44 | 172.7 (9) |
| O21—P1—O20—Mo8 | -64.6 (4) | Eu1—O47—C21—N7 | -167 (2) |
| O19—P1—O20—Mo9 | -64.7 (4) | C23—N7—C21—O47 | -179.5 (9) |
| O22—P1—O20—Mo9 | 175.3 (3) | C22—N7—C21—O47 | 4.0 (14) |
| O21—P1—O20—Mo9 | 55.3 (4) | Eu1—O45—C25—N8 | 176.5 (6) |
| O19—P1—O20—Mo7 | 54.7 (4) | C26—N8—C25—O45 | -7.7 (16) |
| O22—P1—O20—Mo7 | -65.4 (4) | C27—N8—C25—O45 | -177.4 (9) |
| O21—P1—O20—Mo7 | 174.7 (3) | Eu1—O1—C28—N9 | -169.7 (7) |
| O19—P1—O21—Mo10 | 55.4 (4) | C29—N9—C28—O1 | -0.5 (16) |
| O20—P1—O21—Mo10 | -64.9 (3) | C30—N9—C28—O1 | 176.3 (11) |

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

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|-------------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C3—H4 \cdots O31 ⁱ | 0.96 | 2.72 | 3.289 (11) | 118 |
| C4—H7 \cdots O36 ⁱⁱ | 0.96 | 2.61 | 3.476 (12) | 150 |
| C7—H13 \cdots O7 | 0.96 | 2.65 | 3.473 (12) | 145 |
| C8—H15 \cdots O28 ⁱⁱ | 0.96 | 2.51 | 3.316 (13) | 141 |
| C8—H16 \cdots O5 | 0.96 | 2.58 | 3.424 (11) | 147 |
| C10—H18 \cdots O28 ⁱⁱ | 0.93 | 2.62 | 3.516 (10) | 162 |
| C15—H29 \cdots O16 ⁱ | 0.96 | 2.55 | 3.299 (12) | 135 |
| C15—H27 \cdots O32 ⁱⁱⁱ | 0.96 | 2.52 | 3.440 (10) | 160 |
| C15—H28 \cdots O52 ^{iv} | 0.96 | 2.29 | 3.174 (10) | 153 |
| C16—H31 \cdots O6 ⁱⁱⁱ | 0.96 | 2.63 | 3.541 (11) | 159 |
| C22—H41 \cdots O55 | 0.96 | 2.53 | 3.280 (12) | 135 |
| C22—H42 \cdots O11 ^{iv} | 0.96 | 2.45 | 3.305 (11) | 149 |
| C22—H43 \cdots O45 | 0.96 | 2.61 | 3.567 (13) | 172 |
| C23—H44 \cdots O17 ^v | 0.96 | 2.52 | 3.443 (11) | 161 |

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|----------------------------|------|------|------------|-----|
| C25—H55···O24 | 0.93 | 2.53 | 3.337 (11) | 145 |
| C25—H55···O44 | 0.93 | 2.58 | 3.091 (10) | 115 |
| C28—H56···O36 ^v | 0.93 | 2.62 | 3.476 (11) | 153 |
| C30—H60···O36 ^v | 0.96 | 2.58 | 3.458 (14) | 152 |

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