

Tetrakis[μ -3-(3-pyridyl)acrylato- κ^2 O:O']-bis{(1,10-phenanthroline- κ^2 N,N')}[3-(3-pyridyl)acrylato- κ^2 O,O']europium(III) pentahydrate

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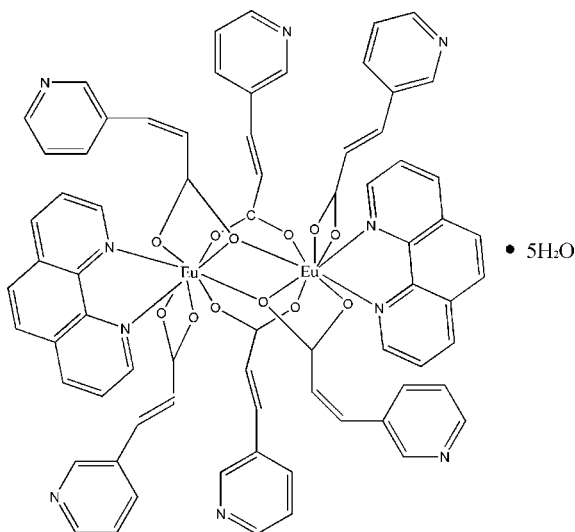
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; disorder in solvent or counterion; R factor = 0.019; wR factor = 0.044; data-to-parameter ratio = 14.1.

The europium^{III} ion in the title compound, $[\text{Eu}_2(\text{C}_8\text{H}_6\text{NO}_2)_6(\text{C}_{12}\text{H}_8\text{N}_2)_2] \cdot 5\text{H}_2\text{O}$, is coordinated by seven carboxylate O atoms and two N atoms from one phenanthroline molecule. The carboxylate groups of 3-(3-pyridyl)acrylate link pairs of europium(III) ions, forming centrosymmetric dinuclear units, which further assemble into a sheet parallel to the (001) plane through hydrogen-bonding interactions involving the uncoordinated water molecules. One water molecule is disordered.

Related literature

For related literature, see: Gunning & Cahill (2005); Liu *et al.* (2006); Ye *et al.* (2005).



Experimental

Crystal data

$[\text{Eu}_2(\text{C}_8\text{H}_6\text{NO}_2)_6(\text{C}_{12}\text{H}_8\text{N}_2)_2] \cdot 5\text{H}_2\text{O}$	$V = 6965.4$ (10) Å ³
$M_r = 1643.24$	$Z = 4$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 25.434$ (2) Å	$\mu = 1.86$ mm ⁻¹
$b = 12.320$ (10) Å	$T = 293$ (2) K
$c = 22.595$ (19) Å	$0.32 \times 0.27 \times 0.13$ mm
$\beta = 100.330$ (10)°	

Data collection

Bruker SMART CCD area-detector diffractometer	25928 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	6480 independent reflections
$T_{\min} = 0.585$, $T_{\max} = 0.791$	5721 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.022$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.019$	460 parameters
$wR(F^2) = 0.044$	H-atom parameters constrained
$S = 1.03$	$\Delta\rho_{\text{max}} = 0.34$ e Å ⁻³
6480 reflections	$\Delta\rho_{\text{min}} = -0.25$ e Å ⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{O1W}-\text{H11W} \cdots \text{O6}$	0.85	1.94	2.775 (3)	171
$\text{O1W}-\text{H12W} \cdots \text{N2}^i$	0.85	2.02	2.856 (3)	167
$\text{O2W}-\text{H21W} \cdots \text{O1W}^{ii}$	0.82	2.48	2.851 (4)	109
$\text{O3W}-\text{H31W} \cdots \text{O2W}^{iii}$	0.82	2.20	2.655 (7)	116

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-III* (Burnett & Johnson, 1996) and *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2276).

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supplementary materials

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Tetrakis[μ -3-(3-pyridyl)acrylato- $\kappa^2 O:O'$]bis{(1,10-phenanthroline- $\kappa^2 N,N'$)[3-(3-pyridyl)acrylato- $\kappa^2 O,O'$]europium(III)} pentahydrate

C.-B. Liu, H.-L. Wen, F. Deng and J.-H. Zuo

Comment

Recently, assembly of high-dimensional supramolecular coordination polymers have attracted considerable attention by exploiting coordination bonds, hydrogen bondings, and π - π stacks [Ye *et al.*, 2005], not only because of their intriguing structural diversity, but also for their potential application as smart optoelectronic, magnetic, and porous materials. 1,10-phenanthroline has been widely used to construct stable supramolecular structures *via* C—H \cdots O or C—H \cdots N hydrogen bonds and π - π stackings, and 3-pyridylacrylic acid (HTPA) is a potential multidentate ligand, (Gunning *et al.*, 2005; Liu *et al.*, 2006). Here, we report the synthesis and structure of a europium supramolecular complex with 3-(3-pyridyl)acrylato and 1,10-phenanthroline, [Eu₂ (C₈H₆NO₂)₆ (C₁₂H₈N₂)₂·(H₂O)₅ (I).

Each Eu^{III} centre is coordinated by seven carboxylate oxygen atoms and two nitrogen atoms from one phenanthroline molecule; the carboxylate groups of 3-(3-pyridyl)acrylato adopt bridging bidentate, chelating and bridging-chelating tridentate modes respectively (Fig. 1). the dihedral angles between them are 59.229 (73), 84.724 (65) and 72.190 (56) ° respectively. The carboxylate groups of 3-(3-pyridyl)acrylato link pairs of europium(III) ions to form dinuclear units, which further build up a sheet parallel to the (0 0 1) plane through hydrogen bondings involving the uncoordinated water molecules (Table 1).

Experimental

A mixture of EuCl₃·6H₂O (0.1 mmol), 3-pyridylacrylic acid (0.1 mmol), 1,10-phenanthroline (0.1 mmol), H₂O (10 ml), and 0.65 M NaOH aqueous solution (0.1 mmol) was sealed in a 25 ml Teflon-lined stainless reactor and heated at 393 K for 72 h under autogenous pressure, then cooled to room temperature, when a few colourless crystals were obtained. Analysis: found C 52.33, H 3.96, N 8.73%; C₇₂H₆₂Eu₂N₁₀O₁₇ requires C 52.01, H 3.85, N 8.43%.

Refinement

All H atoms attached to C atoms were fixed geometrically and treated as riding with C—H = 0.93 Å with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms of water molecule were located in difference Fourier maps and included in the subsequent refinement using restraints (O—H = 0.82 (1) Å and H \cdots H = 1.39 (2) Å) with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. In the last stage of refinement they were treated as riding on their parent O atoms.

Figures

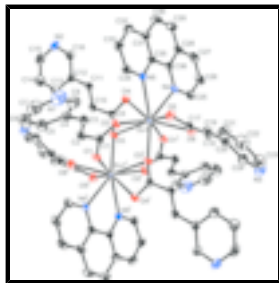


Fig. 1. : The molecular structure of complex (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as small spheres of arbitrary radius. [Symmetry code: (i) 1 - x, 1 - y, 1 - z.]

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Crystal data

[Eu₂(C₈H₆NO₂)₆(C₁₂H₈N₂)₂] \cdot 5H₂O

M_r = 1643.24

Monoclinic, C2/c

Hall symbol: -C 2yc

a = 25.434 (2) Å

b = 12.320 (10) Å

c = 22.595 (19) Å

β = 100.330 (10)°

V = 6965.4 (10) Å³

Z = 4

F_{000} = 3304

D_x = 1.567 Mg m⁻³

Mo $K\alpha$ radiation

λ = 0.71073 Å

Cell parameters from 7048 reflections

θ = 2.7–28.1°

μ = 1.86 mm⁻¹

T = 293 (2) K

Block, colorless

0.32 \times 0.27 \times 0.13 mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

T = 293(2) K

φ and ω scans

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

T_{\min} = 0.585, T_{\max} = 0.791

25928 measured reflections

6480 independent reflections

5721 reflections with $I > 2\sigma(I)$

R_{int} = 0.022

θ_{\max} = 25.5°

θ_{\min} = 2.5°

h = -30→30

k = -14→14

l = -27→27

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)]$ = 0.019

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$wR(F^2) = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.0183P)^2 + 8.1685P]$
$S = 1.03$	where $P = (F_o^2 + 2F_c^2)/3$
6480 reflections	$(\Delta/\sigma)_{\max} = 0.006$
460 parameters	$\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\min} = -0.25 \text{ e } \text{\AA}^{-3}$
	Extinction correction: none

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Eu1	0.528205 (4)	0.611291 (8)	0.562535 (4)	0.02456 (4)	
O5	0.58593 (7)	0.57165 (15)	0.66055 (7)	0.0457 (4)	
O6	0.62759 (6)	0.62061 (13)	0.58772 (7)	0.0417 (4)	
N3	0.82161 (9)	0.3750 (2)	0.77152 (12)	0.0627 (7)	
N4	0.55055 (7)	0.81740 (14)	0.56748 (8)	0.0312 (4)	
N5	0.48983 (7)	0.72683 (15)	0.64279 (8)	0.0311 (4)	
C17	0.62845 (9)	0.58151 (19)	0.63974 (11)	0.0375 (6)	
C18	0.68033 (10)	0.5427 (2)	0.67463 (12)	0.0442 (6)	
H18	0.7110	0.5515	0.6581	0.053*	
C19	0.68467 (10)	0.4966 (2)	0.72778 (11)	0.0430 (6)	
H19	0.6538	0.4954	0.7444	0.052*	
C20	0.73241 (10)	0.4467 (2)	0.76421 (11)	0.0415 (6)	
C21	0.73315 (12)	0.4186 (3)	0.82349 (13)	0.0589 (8)	
H21	0.7035	0.4319	0.8412	0.071*	
C22	0.77820 (14)	0.3705 (3)	0.85628 (14)	0.0729 (10)	
H22	0.7796	0.3521	0.8964	0.087*	
C23	0.82070 (13)	0.3506 (3)	0.82849 (15)	0.0664 (9)	
H23	0.8508	0.3179	0.8509	0.080*	
C24	0.77778 (10)	0.4222 (2)	0.74091 (12)	0.0500 (7)	
H24	0.7777	0.4400	0.7009	0.060*	
C25	0.58064 (10)	0.8617 (2)	0.53183 (11)	0.0418 (6)	
H25	0.5997	0.8160	0.5106	0.050*	
C26	0.58516 (12)	0.9740 (2)	0.52446 (12)	0.0531 (7)	
H26	0.6067	1.0017	0.4988	0.064*	
C27	0.55780 (12)	1.0418 (2)	0.55515 (13)	0.0562 (7)	

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H27	0.5599	1.1165	0.5501	0.067*
C28	0.52609 (10)	0.99896 (19)	0.59464 (12)	0.0450 (6)
C29	0.49626 (13)	1.0650 (2)	0.62910 (15)	0.0629 (8)
H29	0.4973	1.1401	0.6255	0.076*
C30	0.46693 (12)	1.0205 (2)	0.66633 (15)	0.0611 (8)
H30	0.4485	1.0655	0.6886	0.073*
C31	0.46320 (10)	0.9054 (2)	0.67276 (12)	0.0435 (6)
C32	0.43288 (10)	0.8555 (2)	0.71132 (12)	0.0505 (7)
H32	0.4134	0.8978	0.7338	0.061*
C33	0.43197 (10)	0.7457 (2)	0.71572 (11)	0.0472 (6)
H33	0.4124	0.7120	0.7415	0.057*
C34	0.46102 (9)	0.6843 (2)	0.68077 (10)	0.0395 (6)
H34	0.4602	0.6091	0.6842	0.047*
C35	0.49140 (8)	0.83702 (18)	0.63913 (10)	0.0318 (5)
C36	0.52348 (9)	0.88490 (17)	0.59938 (10)	0.0331 (5)
O1	0.44766 (7)	0.35404 (12)	0.53195 (7)	0.0375 (4)
O2	0.47138 (6)	0.48567 (12)	0.60014 (7)	0.0389 (4)
O3	0.44546 (6)	0.55841 (12)	0.47089 (7)	0.0367 (4)
O4	0.44788 (6)	0.71259 (12)	0.51991 (7)	0.0382 (4)
N1	0.40521 (14)	0.2529 (3)	0.83252 (12)	0.0830 (9)
N2	0.21675 (9)	0.92111 (19)	0.44666 (11)	0.0541 (6)
C1	0.44874 (9)	0.39752 (17)	0.58251 (10)	0.0328 (5)
C2	0.42104 (10)	0.33633 (19)	0.62482 (10)	0.0395 (5)
H2	0.3976	0.2814	0.6090	0.047*
C3	0.42757 (10)	0.35487 (19)	0.68318 (11)	0.0390 (6)
H3	0.4495	0.4129	0.6979	0.047*
C4	0.40369 (11)	0.2931 (2)	0.72740 (11)	0.0428 (6)
C5	0.36142 (13)	0.2224 (2)	0.71075 (14)	0.0632 (8)
H5	0.3466	0.2118	0.6704	0.076*
C6	0.34154 (17)	0.1676 (3)	0.75602 (19)	0.0866 (12)
H6	0.3129	0.1199	0.7466	0.104*
C7	0.36502 (18)	0.1855 (3)	0.81466 (18)	0.0882 (12)
H7	0.3516	0.1473	0.8442	0.106*
C8	0.42271 (12)	0.3066 (3)	0.78849 (12)	0.0584 (8)
H8	0.4498	0.3571	0.7997	0.070*
C9	0.42372 (9)	0.64675 (17)	0.48230 (9)	0.0295 (5)
C10	0.36825 (9)	0.67176 (18)	0.45216 (10)	0.0336 (5)
H10	0.3514	0.6266	0.4216	0.040*
C11	0.34228 (9)	0.75715 (18)	0.46803 (10)	0.0346 (5)
H11	0.3607	0.7998	0.4989	0.041*
C12	0.28771 (9)	0.79227 (19)	0.44256 (11)	0.0392 (6)
C13	0.25486 (11)	0.7384 (3)	0.39657 (14)	0.0658 (9)
H13	0.2674	0.6777	0.3789	0.079*
C14	0.20331 (12)	0.7750 (3)	0.37698 (17)	0.0795 (11)
H14	0.1807	0.7390	0.3464	0.095*
C15	0.18612 (11)	0.8654 (3)	0.40342 (15)	0.0651 (9)
H15	0.1512	0.8888	0.3904	0.078*
C16	0.26665 (10)	0.8837 (2)	0.46531 (12)	0.0457 (6)
H16	0.2886	0.9220	0.4956	0.055*

O1W	0.69847 (9)	0.61683 (17)	0.50760 (12)	0.0848 (8)	
H11W	0.6788	0.6122	0.5340	0.127*	
H12W	0.6986	0.5565	0.4895	0.127*	
O2W	0.30658 (11)	0.1792 (3)	0.55009 (14)	0.1219 (11)	
H21W	0.2805	0.2095	0.5594	0.183*	
H22W	0.2973	0.1433	0.5193	0.183*	
O3W	0.3341 (3)	0.9915 (5)	0.6047 (3)	0.133 (2)	0.50
H32W	0.3035	1.0082	0.6078	0.199*	0.50
H31W	0.3521	1.0410	0.5944	0.199*	0.50

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Eu1	0.02668 (6)	0.02120 (6)	0.02471 (6)	−0.00104 (4)	0.00168 (4)	−0.00081 (4)
O5	0.0382 (10)	0.0595 (11)	0.0366 (9)	0.0112 (8)	−0.0010 (8)	0.0015 (8)
O6	0.0356 (9)	0.0442 (10)	0.0416 (10)	−0.0015 (7)	−0.0026 (7)	0.0035 (8)
N3	0.0460 (14)	0.0697 (17)	0.0676 (17)	0.0169 (12)	−0.0031 (12)	0.0009 (13)
N4	0.0331 (10)	0.0262 (10)	0.0332 (10)	−0.0044 (8)	0.0026 (8)	−0.0031 (8)
N5	0.0327 (10)	0.0322 (10)	0.0270 (9)	−0.0002 (8)	0.0018 (8)	−0.0025 (8)
C17	0.0348 (13)	0.0324 (13)	0.0411 (14)	0.0016 (10)	−0.0045 (11)	−0.0092 (10)
C18	0.0327 (13)	0.0459 (15)	0.0499 (15)	0.0015 (11)	−0.0033 (11)	−0.0014 (12)
C19	0.0366 (13)	0.0420 (14)	0.0471 (15)	0.0007 (11)	−0.0016 (11)	−0.0039 (12)
C20	0.0400 (14)	0.0367 (13)	0.0431 (14)	0.0008 (11)	−0.0057 (11)	−0.0026 (11)
C21	0.0577 (18)	0.068 (2)	0.0492 (17)	0.0100 (15)	0.0041 (14)	0.0027 (14)
C22	0.079 (2)	0.084 (2)	0.0483 (18)	0.0120 (19)	−0.0102 (17)	0.0169 (16)
C23	0.0566 (19)	0.0612 (19)	0.070 (2)	0.0155 (15)	−0.0192 (16)	0.0079 (16)
C24	0.0455 (15)	0.0541 (16)	0.0469 (15)	0.0046 (13)	−0.0013 (12)	0.0001 (12)
C25	0.0464 (15)	0.0380 (14)	0.0418 (14)	−0.0111 (11)	0.0102 (11)	−0.0053 (11)
C26	0.0648 (18)	0.0425 (15)	0.0533 (17)	−0.0208 (14)	0.0140 (14)	0.0019 (13)
C27	0.0678 (19)	0.0272 (14)	0.072 (2)	−0.0109 (13)	0.0082 (16)	0.0033 (13)
C28	0.0483 (15)	0.0273 (12)	0.0564 (16)	−0.0001 (11)	0.0012 (12)	−0.0037 (11)
C29	0.070 (2)	0.0292 (14)	0.090 (2)	0.0054 (14)	0.0161 (18)	−0.0103 (15)
C30	0.0621 (19)	0.0410 (16)	0.082 (2)	0.0117 (14)	0.0170 (17)	−0.0203 (15)
C31	0.0387 (14)	0.0424 (15)	0.0483 (15)	0.0069 (11)	0.0048 (11)	−0.0116 (11)
C32	0.0383 (14)	0.0632 (18)	0.0511 (16)	0.0081 (13)	0.0110 (12)	−0.0178 (14)
C33	0.0389 (14)	0.0665 (19)	0.0373 (14)	−0.0032 (13)	0.0099 (11)	−0.0062 (13)
C34	0.0429 (14)	0.0412 (14)	0.0346 (13)	−0.0038 (11)	0.0077 (11)	−0.0019 (10)
C35	0.0298 (11)	0.0306 (12)	0.0322 (12)	0.0016 (9)	−0.0025 (9)	−0.0049 (10)
C36	0.0326 (12)	0.0288 (12)	0.0348 (12)	0.0001 (10)	−0.0024 (9)	−0.0040 (10)
O1	0.0497 (10)	0.0332 (8)	0.0308 (8)	−0.0102 (7)	0.0099 (7)	−0.0043 (7)
O2	0.0511 (10)	0.0324 (9)	0.0353 (9)	−0.0135 (8)	0.0136 (8)	−0.0048 (7)
O3	0.0388 (9)	0.0252 (8)	0.0454 (9)	0.0047 (7)	0.0059 (7)	−0.0021 (7)
O4	0.0359 (9)	0.0310 (8)	0.0426 (9)	0.0043 (7)	−0.0074 (7)	−0.0062 (7)
N1	0.102 (2)	0.097 (2)	0.0588 (17)	0.014 (2)	0.0373 (17)	0.0253 (17)
N2	0.0400 (13)	0.0515 (14)	0.0725 (16)	0.0131 (11)	0.0148 (12)	0.0069 (12)
C1	0.0365 (12)	0.0291 (12)	0.0329 (12)	−0.0023 (10)	0.0064 (10)	0.0012 (10)
C2	0.0475 (14)	0.0341 (13)	0.0392 (13)	−0.0128 (11)	0.0136 (11)	−0.0034 (11)
C3	0.0453 (14)	0.0330 (13)	0.0413 (14)	−0.0038 (11)	0.0145 (11)	0.0005 (10)

supplementary materials

C4	0.0541 (16)	0.0347 (13)	0.0443 (15)	0.0045 (11)	0.0215 (12)	0.0046 (11)
C5	0.085 (2)	0.0511 (18)	0.0599 (19)	-0.0153 (16)	0.0310 (17)	0.0009 (14)
C6	0.110 (3)	0.063 (2)	0.099 (3)	-0.032 (2)	0.053 (3)	0.003 (2)
C7	0.121 (3)	0.080 (3)	0.079 (3)	0.008 (2)	0.060 (3)	0.028 (2)
C8	0.0684 (19)	0.068 (2)	0.0432 (16)	0.0044 (15)	0.0209 (14)	0.0110 (14)
C9	0.0330 (12)	0.0250 (11)	0.0299 (11)	0.0008 (9)	0.0038 (9)	0.0039 (9)
C10	0.0329 (12)	0.0299 (12)	0.0354 (12)	-0.0021 (10)	-0.0011 (10)	-0.0044 (10)
C11	0.0327 (12)	0.0337 (12)	0.0354 (12)	-0.0028 (10)	0.0009 (10)	-0.0018 (10)
C12	0.0321 (13)	0.0388 (13)	0.0456 (14)	0.0026 (10)	0.0045 (11)	0.0012 (11)
C13	0.0437 (16)	0.065 (2)	0.080 (2)	0.0141 (14)	-0.0149 (15)	-0.0226 (17)
C14	0.0462 (18)	0.082 (2)	0.098 (3)	0.0138 (17)	-0.0224 (17)	-0.025 (2)
C15	0.0340 (15)	0.072 (2)	0.085 (2)	0.0112 (14)	-0.0021 (15)	0.0104 (18)
C16	0.0371 (13)	0.0432 (14)	0.0565 (16)	0.0046 (12)	0.0078 (12)	0.0001 (12)
O1W	0.0709 (15)	0.0684 (15)	0.128 (2)	-0.0128 (12)	0.0522 (15)	-0.0190 (14)
O2W	0.093 (2)	0.123 (3)	0.140 (3)	-0.0135 (19)	-0.0045 (19)	0.010 (2)
O3W	0.139 (5)	0.103 (5)	0.133 (5)	-0.017 (4)	-0.036 (4)	0.009 (4)

Geometric parameters (Å, °)

Eu1—O3 ⁱ	2.3604 (15)	C32—H32	0.9300
Eu1—O1 ⁱ	2.3638 (15)	C33—C34	1.397 (3)
Eu1—O2	2.3763 (15)	C33—H33	0.9300
Eu1—O4	2.4400 (15)	C34—H34	0.9300
Eu1—O5	2.4765 (16)	C35—C36	1.443 (3)
Eu1—O6	2.4922 (16)	O1—C1	1.258 (3)
Eu1—N4	2.6001 (18)	O1—Eu1 ⁱ	2.3638 (15)
Eu1—N5	2.6272 (18)	O2—C1	1.260 (3)
Eu1—O3	2.7530 (16)	O3—C9	1.268 (3)
Eu1—C17	2.843 (2)	O3—Eu1 ⁱ	2.3604 (15)
Eu1—C9	2.969 (2)	O4—C9	1.253 (3)
Eu1—Eu1 ⁱ	4.0137 (3)	N1—C7	1.322 (5)
O5—C17	1.260 (3)	N1—C8	1.336 (4)
O6—C17	1.267 (3)	N2—C15	1.327 (4)
N3—C23	1.326 (4)	N2—C16	1.345 (3)
N3—C24	1.335 (3)	C1—C2	1.490 (3)
N4—C25	1.324 (3)	C2—C3	1.319 (3)
N4—C36	1.365 (3)	C2—H2	0.9300
N5—C34	1.332 (3)	C3—C4	1.471 (3)
N5—C35	1.361 (3)	C3—H3	0.9300
C17—C18	1.489 (3)	C4—C5	1.382 (4)
C18—C19	1.315 (3)	C4—C8	1.388 (4)
C18—H18	0.9300	C5—C6	1.394 (4)
C19—C20	1.474 (3)	C5—H5	0.9300
C19—H19	0.9300	C6—C7	1.370 (5)
C20—C21	1.380 (4)	C6—H6	0.9300
C20—C24	1.385 (4)	C7—H7	0.9300
C21—C22	1.381 (4)	C8—H8	0.9300
C21—H21	0.9300	C9—C10	1.485 (3)

C22—C23	1.366 (5)	C10—C11	1.325 (3)
C22—H22	0.9300	C10—H10	0.9300
C23—H23	0.9300	C11—C12	1.469 (3)
C24—H24	0.9300	C11—H11	0.9300
C25—C26	1.400 (3)	C12—C13	1.381 (4)
C25—H25	0.9300	C12—C16	1.385 (3)
C26—C27	1.355 (4)	C13—C14	1.382 (4)
C26—H26	0.9300	C13—H13	0.9300
C27—C28	1.408 (4)	C14—C15	1.371 (4)
C27—H27	0.9300	C14—H14	0.9300
C28—C36	1.412 (3)	C15—H15	0.9300
C28—C29	1.434 (4)	C16—H16	0.9300
C29—C30	1.338 (4)	O1W—H11W	0.8462
C29—H29	0.9300	O1W—H12W	0.8481
C30—C31	1.431 (4)	O2W—H21W	0.8204
C30—H30	0.9300	O2W—H22W	0.8227
C31—C32	1.404 (4)	O3W—H32W	0.8204
C31—C35	1.413 (3)	O3W—H31W	0.8198
C32—C33	1.357 (4)		
O3 ⁱ —Eu1—O1 ⁱ	74.72 (5)	N3—C24—H24	117.5
O3 ⁱ —Eu1—O2	76.31 (5)	C20—C24—H24	117.5
O1 ⁱ —Eu1—O2	135.54 (5)	N4—C25—C26	123.3 (2)
O3 ⁱ —Eu1—O4	126.32 (5)	N4—C25—H25	118.4
O1 ⁱ —Eu1—O4	83.44 (6)	C26—C25—H25	118.4
O2—Eu1—O4	87.38 (6)	C27—C26—C25	119.2 (3)
O3 ⁱ —Eu1—O5	87.40 (6)	C27—C26—H26	120.4
O1 ⁱ —Eu1—O5	129.42 (6)	C25—C26—H26	120.4
O2—Eu1—O5	81.54 (6)	C26—C27—C28	119.9 (2)
O4—Eu1—O5	140.72 (5)	C26—C27—H27	120.1
O3 ⁱ —Eu1—O6	77.26 (5)	C28—C27—H27	120.1
O1 ⁱ —Eu1—O6	77.34 (6)	C27—C28—C36	117.5 (2)
O2—Eu1—O6	127.26 (6)	C27—C28—C29	123.4 (2)
O4—Eu1—O6	144.08 (5)	C36—C28—C29	119.1 (3)
O5—Eu1—O6	52.45 (6)	C30—C29—C28	121.2 (3)
O3 ⁱ —Eu1—N4	143.74 (6)	C30—C29—H29	119.4
O1 ⁱ —Eu1—N4	76.83 (5)	C28—C29—H29	119.4
O2—Eu1—N4	139.73 (5)	C29—C30—C31	121.6 (3)
O4—Eu1—N4	71.25 (5)	C29—C30—H30	119.2
O5—Eu1—N4	93.68 (6)	C31—C30—H30	119.2
O6—Eu1—N4	74.94 (6)	C32—C31—C35	117.5 (2)
O3 ⁱ —Eu1—N5	149.61 (6)	C32—C31—C30	123.4 (2)
O1 ⁱ —Eu1—N5	135.59 (5)	C35—C31—C30	119.1 (3)
O2—Eu1—N5	77.35 (5)	C33—C32—C31	120.0 (2)
O4—Eu1—N5	66.85 (5)	C33—C32—H32	120.0
O5—Eu1—N5	73.95 (6)	C31—C32—H32	120.0
O6—Eu1—N5	107.73 (5)	C32—C33—C34	118.8 (2)

supplementary materials

N4—Eu1—N5	63.04 (6)	C32—C33—H33	120.6
O3 ⁱ —Eu1—O3	76.84 (5)	C34—C33—H33	120.6
O1 ⁱ —Eu1—O3	69.55 (5)	N5—C34—C33	124.0 (2)
O2—Eu1—O3	71.51 (5)	N5—C34—H34	118.0
O4—Eu1—O3	49.54 (5)	C33—C34—H34	118.0
O5—Eu1—O3	151.25 (6)	N5—C35—C31	122.6 (2)
O6—Eu1—O3	142.18 (5)	N5—C35—C36	118.14 (19)
N4—Eu1—O3	113.28 (5)	C31—C35—C36	119.3 (2)
N5—Eu1—O3	108.60 (5)	N4—C36—C28	122.1 (2)
O3 ⁱ —Eu1—C17	78.89 (6)	N4—C36—C35	118.33 (19)
O1 ⁱ —Eu1—C17	103.18 (7)	C28—C36—C35	119.6 (2)
O2—Eu1—C17	103.45 (7)	C1—O1—Eu1 ⁱ	140.95 (14)
O4—Eu1—C17	154.62 (6)	C1—O2—Eu1	136.14 (14)
O5—Eu1—C17	26.26 (6)	C9—O3—Eu1 ⁱ	169.88 (14)
O6—Eu1—C17	26.44 (6)	C9—O3—Eu1	86.92 (12)
N4—Eu1—C17	86.25 (6)	Eu1 ⁱ —O3—Eu1	103.16 (5)
N5—Eu1—C17	92.85 (6)	C9—O4—Eu1	102.16 (13)
O3—Eu1—C17	155.71 (6)	C7—N1—C8	115.2 (3)
O3 ⁱ —Eu1—C9	102.08 (6)	C15—N2—C16	116.7 (2)
O1 ⁱ —Eu1—C9	76.75 (6)	O1—C1—O2	126.1 (2)
O2—Eu1—C9	77.23 (6)	O1—C1—C2	115.56 (19)
O4—Eu1—C9	24.37 (5)	O2—C1—C2	118.4 (2)
O5—Eu1—C9	153.82 (6)	C3—C2—C1	124.4 (2)
O6—Eu1—C9	153.25 (6)	C3—C2—H2	117.8
N4—Eu1—C9	92.72 (6)	C1—C2—H2	117.8
N5—Eu1—C9	86.51 (6)	C2—C3—C4	126.6 (2)
O3—Eu1—C9	25.25 (5)	C2—C3—H3	116.7
C17—Eu1—C9	178.95 (6)	C4—C3—H3	116.7
O3 ⁱ —Eu1—Eu1 ⁱ	41.90 (4)	C5—C4—C8	117.5 (2)
O1 ⁱ —Eu1—Eu1 ⁱ	66.76 (4)	C5—C4—C3	122.5 (2)
O2—Eu1—Eu1 ⁱ	69.10 (4)	C8—C4—C3	120.0 (2)
O4—Eu1—Eu1 ⁱ	84.45 (4)	C4—C5—C6	118.2 (3)
O5—Eu1—Eu1 ⁱ	125.08 (4)	C4—C5—H5	120.9
O6—Eu1—Eu1 ⁱ	114.34 (4)	C6—C5—H5	120.9
N4—Eu1—Eu1 ⁱ	138.18 (4)	C7—C6—C5	118.6 (3)
N5—Eu1—Eu1 ⁱ	136.55 (4)	C7—C6—H6	120.7
O3—Eu1—Eu1 ⁱ	34.93 (3)	C5—C6—H6	120.7
C17—Eu1—Eu1 ⁱ	120.79 (5)	N1—C7—C6	125.1 (3)
C9—Eu1—Eu1 ⁱ	60.18 (4)	N1—C7—H7	117.4
C17—O5—Eu1	93.33 (14)	C6—C7—H7	117.4
C17—O6—Eu1	92.42 (14)	N1—C8—C4	125.3 (3)
C23—N3—C24	116.3 (3)	N1—C8—H8	117.4
C25—N4—C36	118.12 (19)	C4—C8—H8	117.4
C25—N4—Eu1	121.48 (15)	O4—C9—O3	120.99 (19)
C36—N4—Eu1	119.38 (14)	O4—C9—C10	119.13 (19)

C34—N5—C35	117.2 (2)	O3—C9—C10	119.86 (19)
C34—N5—Eu1	123.15 (15)	O4—C9—Eu1	53.47 (10)
C35—N5—Eu1	118.67 (14)	O3—C9—Eu1	67.83 (11)
O5—C17—O6	120.7 (2)	C10—C9—Eu1	169.61 (15)
O5—C17—C18	120.6 (2)	C11—C10—C9	121.3 (2)
O6—C17—C18	118.6 (2)	C11—C10—H10	119.4
O5—C17—Eu1	60.41 (12)	C9—C10—H10	119.4
O6—C17—Eu1	61.14 (12)	C10—C11—C12	127.6 (2)
C18—C17—Eu1	168.00 (16)	C10—C11—H11	116.2
C19—C18—C17	122.9 (2)	C12—C11—H11	116.2
C19—C18—H18	118.5	C13—C12—C16	116.6 (2)
C17—C18—H18	118.5	C13—C12—C11	123.7 (2)
C18—C19—C20	128.0 (3)	C16—C12—C11	119.7 (2)
C18—C19—H19	116.0	C12—C13—C14	119.7 (3)
C20—C19—H19	116.0	C12—C13—H13	120.2
C21—C20—C24	116.6 (2)	C14—C13—H13	120.2
C21—C20—C19	120.9 (2)	C15—C14—C13	119.0 (3)
C24—C20—C19	122.5 (2)	C15—C14—H14	120.5
C20—C21—C22	119.6 (3)	C13—C14—H14	120.5
C20—C21—H21	120.2	N2—C15—C14	123.4 (3)
C22—C21—H21	120.2	N2—C15—H15	118.3
C23—C22—C21	118.6 (3)	C14—C15—H15	118.3
C23—C22—H22	120.7	N2—C16—C12	124.6 (3)
C21—C22—H22	120.7	N2—C16—H16	117.7
N3—C23—C22	123.9 (3)	C12—C16—H16	117.7
N3—C23—H23	118.0	H11W—O1W—H12W	109.4
C22—C23—H23	118.0	H21W—O2W—H22W	109.8
N3—C24—C20	125.0 (3)	H32W—O3W—H31W	115.1

Symmetry codes: (i) $-x+1, -y+1, -z+1$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H11W \cdots O6	0.85	1.94	2.775 (3)	171
O1W—H12W \cdots N2 ⁱⁱ	0.85	2.02	2.856 (3)	167
O2W—H21W \cdots O1W ⁱⁱⁱ	0.82	2.48	2.851 (4)	109
O3W—H31W \cdots O2W ^{iv}	0.82	2.20	2.655 (7)	116

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

Fig. 1

