

catena-Poly[tris(μ_2 -1H-benzimidazole-5-carboxylato)europium(III)]

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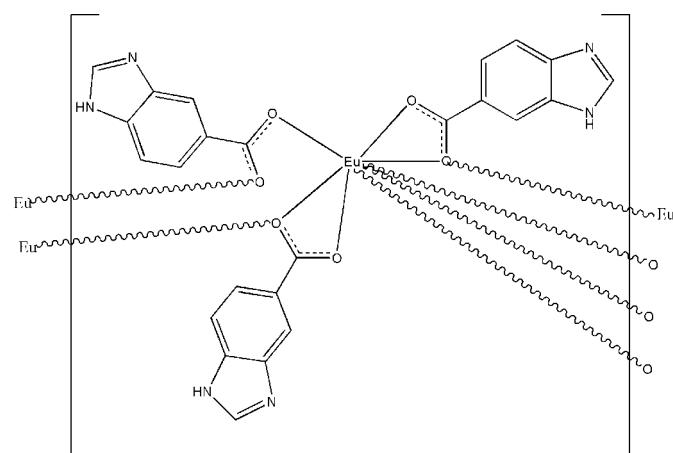
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Key indicators: single-crystal X-ray study; $T = 293\text{ K}$; mean $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$; R factor = 0.022; wR factor = 0.054; data-to-parameter ratio = 10.7.

In the title one-dimensional coordination polymer, $[\text{Eu}(\text{C}_8\text{H}_5\text{N}_2\text{O}_2)_3]_n$, the Eu^{III} ion is eight-coordinated by the carboxylate O atoms of six ligands in a distorted monocapped pentagonal-bipyramidal geometry. The ligands link Eu^{III} ions, forming helical chains parallel to the c axis, with $\text{Eu}\cdots\text{Eu}$ separations of $4.0678(11)\text{ \AA}$. The chains are further interconnected by $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonds into a three-dimensional supramolecular network. The crystal studied was a racemic twin, as suggested by the Flack parameter of 0.367 (14).

Related literature

For general background to coordination polymers based on *N*-heterocyclic carboxylates, see: Huang *et al.* (2009); Cheng *et al.* (2008); Qiu *et al.* (2007). For related structures, see: Guo, Cao *et al.* (2007); Guo, Li *et al.* (2007); Peng *et al.* (2010).



Experimental

Crystal data

$[\text{Eu}(\text{C}_8\text{H}_5\text{N}_2\text{O}_2)_3]$	$V = 2233.1(4)\text{ \AA}^3$
$M_r = 635.38$	$Z = 4$
Monoclinic, Cc	$\text{Mo } K\alpha$ radiation
$a = 23.211(2)\text{ \AA}$	$\mu = 2.87\text{ mm}^{-1}$
$b = 12.4312(12)\text{ \AA}$	$T = 293\text{ K}$
$c = 8.1329(8)\text{ \AA}$	$0.20 \times 0.19 \times 0.13\text{ mm}$
$\beta = 107.902(1)^{\circ}$	

Data collection

Bruker APEXII area-detector diffractometer	5623 measured reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 2008)	3595 independent reflections
$T_{\min} = 0.598$, $T_{\max} = 0.707$	3412 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.022$	H-atom parameters constrained
$wR(F^2) = 0.054$	$\Delta\rho_{\max} = 1.07\text{ e \AA}^{-3}$
$S = 1.05$	$\Delta\rho_{\min} = -0.66\text{ e \AA}^{-3}$
3595 reflections	Absolute structure: Flack (1983),
335 parameters	1587 Friedel pairs
2 restraints	Flack parameter: 0.367 (14)

Table 1
Hydrogen-bond geometry (\AA , $^{\circ}$).

$D-\text{H}\cdots\text{A}$	$D-\text{H}$	$\text{H}\cdots\text{A}$	$D\cdots\text{A}$	$D-\text{H}\cdots\text{A}$
$\text{N}3-\text{H}3\text{A}\cdots\text{N}2^{\text{i}}$	0.86	1.96	2.798 (6)	165
$\text{N}5-\text{H}5\cdots\text{N}4^{\text{ii}}$	0.86	2.04	2.839 (6)	155
$\text{N}1-\text{H}1\cdots\text{N}6^{\text{ii}}$	0.86	1.97	2.827 (6)	173

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: RZ2533).

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Comment

Metal coordination polymers based on N-heterocyclic carboxylates such as pyridinecarboxylates have raised intense interest for their structural diversity and their potential applications as functional materials (Huang *et al.*, 2009; Cheng *et al.*, 2008; Qiu *et al.*, 2007). To date, one-, two-, and three-dimensional coordination polymers have been synthesized by the choice of appropriate metal ions and versatile benzimidazole carboxylates as ligands (Guo, Cao *et al.*, 2007; Guo, Li *et al.*, 2007b; Peng *et al.*, 2010). Herein, the hydrothermal treatment of Eu₂O₃ with 1H-benzimidazole-5-carboxylic acid led to a the synthesis of the novel title compound, [Eu(C₈H₅N₂O₂)₃]_n, whose structure is reported herein.

As depicted in Fig. 1, the europium(III) ion is eight-coordinated by the O atoms of six 1H-benzimidazole-5-carboxylate ligands, adopting a distorted monocapped pentagonal-bipyramidal geometry. The 1H-benzimidazole-5-carboxylate ligands link europium ions, forming helical chains parallel to the *c* axis. The Eu–Eu separations within the polymer are 4.0678 (11) Å. These chains are further interconnected by N—H···N hydrogen bonds and extend to form a three-dimensional supramolecular network (Table 1; Fig. 2).

Experimental

A mixture of Eu₂O₃ (0.070 g, 0.2 mmol), 1H-benzimidazole-5-carboxylic acid (0.193 g, 1.2 mmol), and H₂O (10 mL) was sealed in a 20 mL Teflon-lined reactor, which was heated in an oven to 423 K for 48 h and then cooled to room temperature at a rate of 5 K h⁻¹. Colourless crystals suitable for X-ray analysis were obtained in a yield of 76% based on Eu.

Refinement

The crystal studied was a racemic twin, as suggested by the Flack parameter of 0.367 (14) obtained by the TWIN/BASF procedure in SHELXL (Sheldrick, 2008). All H atoms were fixed geometrically and treated as riding, with C—H = 0.93 Å, N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C, N).

Figures

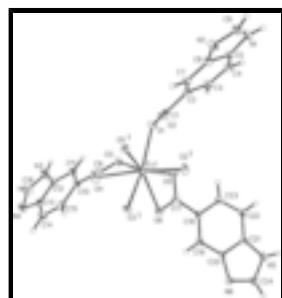


Fig. 1. The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids. Symmetry code: (i) x, -y, 0.5+z.

supplementary materials

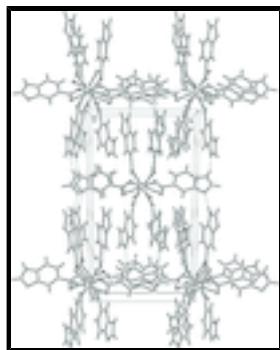


Fig. 2. Crystal packing of the title compound viewed along the c axis. Intermolecular hydrogen bonds are shown as dashed lines.

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Crystal data

[Eu(C ₈ H ₅ N ₂ O ₂) ₃]	$F(000) = 1248$
$M_r = 635.38$	$D_x = 1.890 \text{ Mg m}^{-3}$
Monoclinic, Cc	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: C -2yc	Cell parameters from 2300 reflections
$a = 23.211 (2) \text{ \AA}$	$\theta = 1.2\text{--}28.0^\circ$
$b = 12.4312 (12) \text{ \AA}$	$\mu = 2.87 \text{ mm}^{-1}$
$c = 8.1329 (8) \text{ \AA}$	$T = 293 \text{ K}$
$\beta = 107.902 (1)^\circ$	Block, colourless
$V = 2233.1 (4) \text{ \AA}^3$	$0.20 \times 0.19 \times 0.13 \text{ mm}$
$Z = 4$	

Data collection

Bruker APEXII area-detector diffractometer	3595 independent reflections
Radiation source: fine-focus sealed tube graphite	3412 reflections with $I > 2\sigma(I)$
ϕ and ω scans	$R_{\text{int}} = 0.019$
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 2008)	$\theta_{\text{max}} = 25.2^\circ$, $\theta_{\text{min}} = 1.8^\circ$
$T_{\text{min}} = 0.598$, $T_{\text{max}} = 0.707$	$h = -27 \rightarrow 27$
5623 measured reflections	$k = -12 \rightarrow 14$
	$l = -9 \rightarrow 9$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.022$	H-atom parameters constrained
$wR(F^2) = 0.054$	$w = 1/[\sigma^2(F_o^2) + (0.0245P)^2 + 1.858P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
	$(\Delta/\sigma)_{\text{max}} < 0.001$

3595 reflections	$\Delta\rho_{\max} = 1.07 \text{ e \AA}^{-3}$
335 parameters	$\Delta\rho_{\min} = -0.66 \text{ e \AA}^{-3}$
2 restraints	Absolute structure: Flack (1983), 1587 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.367 (14)

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 $F^2 > 2\text{sigma}(F^2)$ 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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.7810 (2)	-0.1030 (3)	0.3121 (6)	0.0246 (10)
C2	0.7133 (2)	-0.1136 (3)	0.2747 (6)	0.0247 (10)
C3	0.6748 (2)	-0.0808 (4)	0.1122 (7)	0.0320 (11)
H3	0.6914	-0.0568	0.0285	0.038*
C4	0.6124 (2)	-0.0839 (4)	0.0754 (7)	0.0350 (12)
H4	0.5869	-0.0602	-0.0305	0.042*
C5	0.58948 (19)	-0.1233 (4)	0.2012 (6)	0.0262 (10)
C6	0.6284 (2)	-0.1580 (4)	0.3601 (6)	0.0266 (10)
C7	0.69065 (19)	-0.1513 (4)	0.3995 (6)	0.0260 (10)
H7	0.7161	-0.1717	0.5074	0.031*
C8	0.5362 (2)	-0.1815 (4)	0.3580 (7)	0.0379 (12)
H8	0.5029	-0.2007	0.3920	0.045*
C9	0.9849 (2)	-0.0888 (3)	0.5739 (6)	0.0250 (10)
C10	1.0465 (2)	-0.1076 (3)	0.5592 (6)	0.0235 (10)
C11	1.0547 (2)	-0.1516 (4)	0.4114 (6)	0.0268 (10)
H11	1.0219	-0.1689	0.3161	0.032*
C12	1.1136 (2)	-0.1687 (4)	0.4115 (6)	0.0266 (10)
C13	1.16339 (19)	-0.1397 (4)	0.5542 (6)	0.0272 (10)
C14	1.1553 (2)	-0.0948 (4)	0.7007 (7)	0.0355 (12)
H14	1.1882	-0.0749	0.7940	0.043*
C15	1.0968 (2)	-0.0804 (4)	0.7041 (6)	0.0333 (12)
H15	1.0902	-0.0525	0.8027	0.040*
C16	1.1963 (2)	-0.2119 (5)	0.3592 (8)	0.0470 (15)
H16	1.2226	-0.2391	0.3033	0.056*
C17	0.88812 (19)	0.1921 (3)	0.4501 (6)	0.0238 (11)
C18	0.8756 (2)	0.3027 (4)	0.3823 (7)	0.0235 (12)
C19	0.9090 (2)	0.3881 (4)	0.4713 (7)	0.0248 (11)

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H19	0.9418	0.3766	0.5697	0.030*
C20	0.8928 (5)	0.4911 (4)	0.411 (2)	0.0215 (18)
C21	0.8393 (2)	0.5091 (3)	0.2693 (7)	0.0246 (11)
C22	0.8063 (2)	0.4221 (4)	0.1781 (6)	0.0289 (11)
H22	0.7722	0.4332	0.0834	0.035*
C23	0.8256 (2)	0.3205 (4)	0.2321 (6)	0.0285 (11)
H23	0.8056	0.2618	0.1690	0.034*
C24	0.8778 (3)	0.6620 (4)	0.3649 (7)	0.0335 (16)
H24	0.8834	0.7360	0.3760	0.040*
Eu1	0.88497 (4)	0.004139 (14)	0.65258 (9)	0.01831 (7)
N1	0.53063 (17)	-0.1384 (3)	0.2059 (6)	0.0357 (10)
H1	0.4976	-0.1229	0.1264	0.043*
N2	0.59260 (17)	-0.1958 (4)	0.4594 (6)	0.0347 (10)
N3	1.13677 (18)	-0.2146 (4)	0.2901 (6)	0.0388 (10)
H3A	1.1166	-0.2396	0.1904	0.047*
N4	1.21553 (18)	-0.1670 (3)	0.5153 (6)	0.0372 (10)
N5	0.83136 (19)	0.6180 (3)	0.2483 (6)	0.0307 (10)
H5	0.8021	0.6508	0.1742	0.037*
N6	0.91641 (18)	0.5911 (3)	0.4667 (6)	0.0296 (9)
O1	0.81272 (13)	-0.1030 (3)	0.4680 (4)	0.0293 (7)
O2	0.80206 (14)	-0.0948 (3)	0.1870 (4)	0.0340 (8)
O3	0.93970 (13)	-0.0700 (3)	0.4411 (4)	0.0257 (7)
O4	0.97779 (16)	-0.0890 (3)	0.7212 (4)	0.0416 (9)
O5	0.86050 (14)	0.1111 (2)	0.3630 (4)	0.0240 (7)
O6	0.92350 (15)	0.1775 (2)	0.6017 (4)	0.0302 (7)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.025 (2)	0.022 (2)	0.030 (3)	-0.0051 (18)	0.013 (2)	-0.0025 (18)
C2	0.017 (2)	0.024 (2)	0.031 (3)	-0.0055 (17)	0.005 (2)	-0.0043 (18)
C3	0.032 (3)	0.036 (3)	0.029 (3)	-0.006 (2)	0.012 (2)	0.007 (2)
C4	0.034 (3)	0.040 (3)	0.027 (3)	0.002 (2)	0.003 (2)	0.007 (2)
C5	0.016 (2)	0.031 (2)	0.027 (3)	0.0007 (19)	0.001 (2)	-0.0004 (19)
C6	0.021 (2)	0.033 (3)	0.027 (3)	0.0007 (19)	0.008 (2)	0.000 (2)
C7	0.018 (2)	0.033 (3)	0.025 (3)	-0.0010 (18)	0.004 (2)	0.0056 (19)
C8	0.023 (3)	0.049 (3)	0.044 (3)	-0.003 (2)	0.016 (2)	-0.007 (3)
C9	0.024 (2)	0.025 (2)	0.024 (3)	0.0073 (19)	0.004 (2)	0.0018 (19)
C10	0.017 (2)	0.026 (2)	0.027 (3)	0.0025 (18)	0.005 (2)	-0.0010 (18)
C11	0.017 (2)	0.032 (2)	0.030 (3)	0.0000 (19)	0.005 (2)	-0.003 (2)
C12	0.024 (2)	0.030 (2)	0.025 (3)	-0.0008 (19)	0.006 (2)	-0.0020 (19)
C13	0.014 (2)	0.029 (2)	0.037 (3)	0.0010 (18)	0.005 (2)	0.000 (2)
C14	0.022 (3)	0.041 (3)	0.036 (3)	-0.001 (2)	-0.002 (2)	-0.013 (2)
C15	0.033 (3)	0.035 (3)	0.028 (3)	0.007 (2)	0.004 (2)	-0.011 (2)
C16	0.033 (3)	0.065 (4)	0.053 (4)	0.003 (3)	0.027 (3)	-0.007 (3)
C17	0.021 (2)	0.028 (2)	0.029 (3)	0.0003 (19)	0.018 (2)	-0.0008 (19)
C18	0.019 (3)	0.026 (2)	0.029 (3)	0.002 (2)	0.012 (3)	0.001 (2)
C19	0.018 (3)	0.028 (3)	0.028 (3)	0.000 (2)	0.005 (2)	0.001 (2)

C20	0.014 (5)	0.022 (2)	0.028 (3)	0.003 (2)	0.007 (4)	0.007 (2)
C21	0.016 (3)	0.030 (3)	0.026 (3)	0.0005 (17)	0.005 (2)	0.0037 (18)
C22	0.021 (2)	0.036 (3)	0.026 (3)	0.001 (2)	0.001 (2)	0.004 (2)
C23	0.022 (2)	0.034 (3)	0.028 (3)	-0.006 (2)	0.005 (2)	-0.006 (2)
C24	0.030 (4)	0.024 (3)	0.048 (5)	0.003 (3)	0.014 (4)	0.007 (3)
Eu1	0.01663 (10)	0.02304 (10)	0.01675 (10)	0.00095 (12)	0.00732 (7)	0.00014 (12)
N1	0.016 (2)	0.048 (3)	0.039 (3)	0.0046 (18)	0.0030 (19)	0.002 (2)
N2	0.021 (2)	0.052 (3)	0.035 (3)	-0.0045 (19)	0.0135 (19)	0.002 (2)
N3	0.022 (2)	0.064 (3)	0.031 (3)	0.003 (2)	0.0091 (18)	-0.009 (2)
N4	0.021 (2)	0.049 (3)	0.044 (3)	-0.0021 (19)	0.012 (2)	-0.007 (2)
N5	0.024 (2)	0.029 (2)	0.037 (3)	0.0042 (18)	0.005 (2)	0.0062 (18)
N6	0.026 (2)	0.022 (2)	0.040 (3)	-0.0045 (17)	0.009 (2)	-0.0010 (18)
O1	0.0202 (17)	0.0360 (19)	0.029 (2)	-0.0072 (14)	0.0032 (15)	-0.0032 (14)
O2	0.0261 (18)	0.043 (2)	0.034 (2)	-0.0138 (15)	0.0119 (16)	-0.0060 (16)
O3	0.0183 (17)	0.0327 (18)	0.0256 (18)	0.0060 (13)	0.0063 (14)	0.0054 (14)
O4	0.0321 (19)	0.069 (3)	0.026 (2)	0.0199 (18)	0.0120 (16)	0.0046 (17)
O5	0.0285 (17)	0.0204 (16)	0.0230 (17)	-0.0002 (13)	0.0080 (14)	-0.0008 (13)
O6	0.0311 (18)	0.0283 (17)	0.0244 (19)	-0.0013 (14)	-0.0016 (15)	0.0049 (14)

Geometric parameters (Å, °)

C1—O1	1.255 (5)	C16—H16	0.9300
C1—O2	1.261 (5)	C17—O6	1.267 (5)
C1—C2	1.511 (6)	C17—O5	1.283 (5)
C2—C7	1.363 (6)	C17—C18	1.477 (6)
C2—C3	1.409 (7)	C18—C19	1.381 (7)
C3—C4	1.385 (7)	C18—C23	1.420 (7)
C3—H3	0.9300	C19—C20	1.381 (8)
C4—C5	1.381 (7)	C19—H19	0.9300
C4—H4	0.9300	C20—N6	1.377 (9)
C5—N1	1.391 (6)	C20—C21	1.428 (13)
C5—C6	1.398 (6)	C21—N5	1.370 (6)
C6—C7	1.383 (6)	C21—C22	1.399 (7)
C6—N2	1.406 (6)	C22—C23	1.367 (6)
C7—H7	0.9300	C22—H22	0.9300
C8—N1	1.317 (7)	C23—H23	0.9300
C8—N2	1.327 (6)	C24—N5	1.316 (7)
C8—H8	0.9300	C24—N6	1.346 (7)
C9—O4	1.258 (5)	C24—H24	0.9300
C9—O3	1.275 (5)	Eu1—O1	2.300 (3)
C9—C10	1.491 (6)	Eu1—O2 ⁱ	2.320 (3)
C10—C11	1.385 (7)	Eu1—O4	2.357 (3)
C10—C15	1.421 (6)	Eu1—O6	2.417 (3)
C11—C12	1.384 (6)	Eu1—O5 ⁱ	2.429 (3)
C11—H11	0.9300	Eu1—O3 ⁱ	2.441 (3)
C12—N3	1.384 (6)	Eu1—O3	2.601 (3)
C12—C13	1.410 (6)	Eu1—O5	2.610 (3)
C13—C14	1.380 (7)	N1—H1	0.8600

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C13—N4	1.384 (6)	N3—H3A	0.8600
C14—C15	1.376 (7)	N5—H5	0.8600
C14—H14	0.9300	O2—Eu1 ⁱⁱ	2.320 (3)
C15—H15	0.9300	O3—Eu1 ⁱⁱ	2.441 (3)
C16—N3	1.322 (6)	O5—Eu1 ⁱⁱ	2.429 (3)
C16—N4	1.332 (7)		
O1—C1—O2	124.2 (4)	N5—C24—H24	122.8
O1—C1—C2	117.0 (4)	N6—C24—H24	122.8
O2—C1—C2	118.8 (4)	O1—Eu1—O2 ⁱ	83.94 (12)
C7—C2—C3	121.2 (4)	O1—Eu1—O4	107.47 (13)
C7—C2—C1	119.7 (4)	O2 ⁱ —Eu1—O4	160.37 (12)
C3—C2—C1	119.0 (4)	O1—Eu1—O6	129.67 (12)
C4—C3—C2	121.0 (4)	O2 ⁱ —Eu1—O6	87.25 (11)
C4—C3—H3	119.5	O4—Eu1—O6	96.84 (13)
C2—C3—H3	119.5	O1—Eu1—O5 ⁱ	80.62 (11)
C5—C4—C3	117.7 (5)	O2 ⁱ —Eu1—O5 ⁱ	79.58 (11)
C5—C4—H4	121.1	O4—Eu1—O5 ⁱ	86.46 (12)
C3—C4—H4	121.1	O6—Eu1—O5 ⁱ	145.61 (11)
C4—C5—N1	132.4 (4)	O1—Eu1—O3 ⁱ	151.78 (11)
C4—C5—C6	120.5 (4)	O2 ⁱ —Eu1—O3 ⁱ	85.82 (12)
N1—C5—C6	107.1 (4)	O4—Eu1—O3 ⁱ	76.66 (12)
C7—C6—C5	121.9 (4)	O6—Eu1—O3 ⁱ	75.81 (11)
C7—C6—N2	130.3 (5)	O5 ⁱ —Eu1—O3 ⁱ	71.68 (10)
C5—C6—N2	107.8 (4)	O1—Eu1—O3	76.68 (11)
C2—C7—C6	117.6 (4)	O2 ⁱ —Eu1—O3	147.53 (12)
C2—C7—H7	121.2	O4—Eu1—O3	52.10 (11)
C6—C7—H7	121.2	O6—Eu1—O3	85.47 (11)
N1—C8—N2	115.6 (5)	O5 ⁱ —Eu1—O3	121.64 (11)
N1—C8—H8	122.2	O3 ⁱ —Eu1—O3	122.60 (13)
N2—C8—H8	122.2	O1—Eu1—O5	78.07 (11)
O4—C9—O3	119.5 (4)	O2 ⁱ —Eu1—O5	84.43 (11)
O4—C9—C10	119.1 (4)	O4—Eu1—O5	113.16 (11)
O3—C9—C10	121.4 (4)	O6—Eu1—O5	51.75 (10)
C11—C10—C15	121.1 (4)	O5 ⁱ —Eu1—O5	154.53 (14)
C11—C10—C9	121.5 (4)	O3 ⁱ —Eu1—O5	126.96 (10)
C15—C10—C9	117.4 (4)	O3—Eu1—O5	66.35 (10)
C12—C11—C10	117.3 (4)	O1—Eu1—Eu1 ⁱ	114.44 (9)
C12—C11—H11	121.3	O2 ⁱ —Eu1—Eu1 ⁱ	68.71 (9)
C10—C11—H11	121.3	O4—Eu1—Eu1 ⁱ	91.82 (9)
C11—C12—N3	131.6 (4)	O6—Eu1—Eu1 ⁱ	107.90 (8)
C11—C12—C13	121.4 (4)	O5 ⁱ —Eu1—Eu1 ⁱ	37.71 (7)
N3—C12—C13	107.0 (4)	O3 ⁱ —Eu1—Eu1 ⁱ	37.56 (7)
C14—C13—N4	131.1 (4)	O3—Eu1—Eu1 ⁱ	143.34 (7)

C14—C13—C12	121.3 (4)	O5—Eu1—Eu1 ⁱ	147.99 (6)
N4—C13—C12	107.6 (4)	O1—Eu1—Eu1 ⁱⁱ	63.70 (9)
C15—C14—C13	117.8 (5)	O2 ⁱ —Eu1—Eu1 ⁱⁱ	112.81 (9)
C15—C14—H14	121.1	O4—Eu1—Eu1 ⁱⁱ	86.75 (9)
C13—C14—H14	121.1	O6—Eu1—Eu1 ⁱⁱ	74.80 (8)
C14—C15—C10	121.1 (4)	O5 ⁱ —Eu1—Eu1 ⁱⁱ	139.58 (7)
C14—C15—H15	119.5	O3 ⁱ —Eu1—Eu1 ⁱⁱ	144.06 (7)
C10—C15—H15	119.5	O3—Eu1—Eu1 ⁱⁱ	34.90 (7)
N3—C16—N4	114.6 (5)	O5—Eu1—Eu1 ⁱⁱ	34.69 (6)
N3—C16—H16	122.7	Eu1 ⁱ —Eu1—Eu1 ⁱⁱ	177.100 (10)
N4—C16—H16	122.7	C8—N1—C5	105.5 (4)
O6—C17—O5	119.3 (4)	C8—N1—H1	127.3
O6—C17—C18	119.4 (4)	C5—N1—H1	127.3
O5—C17—C18	121.2 (4)	C8—N2—C6	104.0 (4)
C19—C18—C23	120.6 (4)	C16—N3—C12	105.7 (4)
C19—C18—C17	120.4 (5)	C16—N3—H3A	127.2
C23—C18—C17	118.7 (4)	C12—N3—H3A	127.2
C20—C19—C18	118.6 (7)	C16—N4—C13	105.1 (4)
C20—C19—H19	120.7	C24—N5—C21	105.7 (4)
C18—C19—H19	120.7	C24—N5—H5	127.1
N6—C20—C19	133.0 (11)	C21—N5—H5	127.1
N6—C20—C21	106.4 (5)	C24—N6—C20	105.5 (6)
C19—C20—C21	120.4 (8)	C1—O1—Eu1	137.9 (3)
N5—C21—C22	131.8 (5)	C1—O2—Eu1 ⁱⁱ	132.7 (3)
N5—C21—C20	107.9 (4)	C9—O3—Eu1 ⁱⁱ	157.8 (3)
C22—C21—C20	120.4 (4)	C9—O3—Eu1	86.9 (3)
C23—C22—C21	118.2 (5)	Eu1 ⁱⁱ —O3—Eu1	107.53 (11)
C23—C22—H22	120.9	C9—O4—Eu1	98.7 (3)
C21—C22—H22	120.9	C17—O5—Eu1 ⁱⁱ	131.8 (3)
C22—C23—C18	121.4 (4)	C17—O5—Eu1	88.2 (2)
C22—C23—H23	119.3	Eu1 ⁱⁱ —O5—Eu1	107.59 (11)
C18—C23—H23	119.3	C17—O6—Eu1	97.5 (3)
N5—C24—N6	114.5 (5)		

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

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

$D\cdots H$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
N3—H3A ⁱⁱⁱ —N2 ⁱⁱⁱ	0.86	1.96	2.798 (6)	165.
N5—H5 ^{iv} —N4 ^{iv}	0.86	2.04	2.839 (6)	155.
N1—H1 ^{iv} —N6 ^{iv}	0.86	1.97	2.827 (6)	173.

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

supplementary materials

Fig. 1

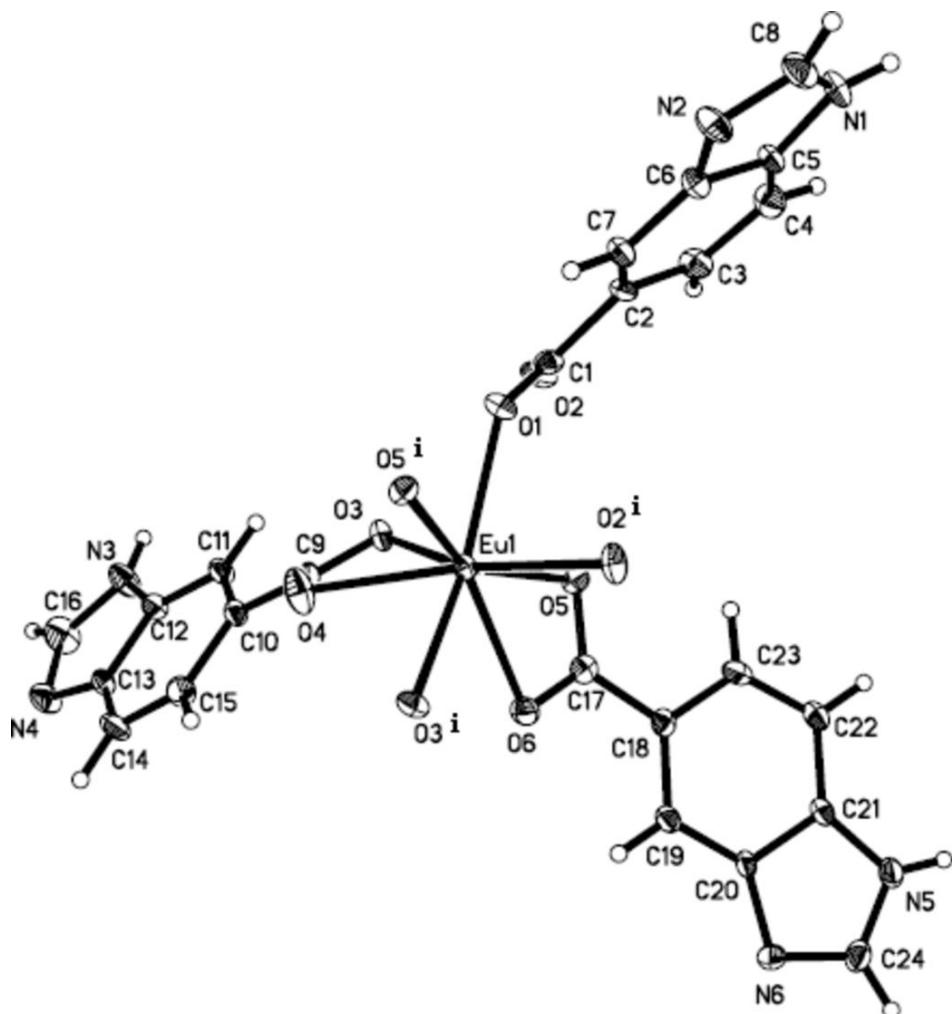


Fig. 2

