

Retraction of articles by H. Zhong *et al.*

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A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *et al.* are retracted. Full details of all the articles are given in Table 1.

**Table 1**

Details of articles to be retracted, in order of publication.

| Title  | Reference                            | DOI                       | Refcode  |
|--|--------------------------------------|---------------------------|----------|
| <i>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate</i>  | Zhong, Zeng, Liu & Luo (2006a)       | 10.1107/S1600536806041122 | KERQEE   |
| <i>cis-Dichlorobis(1,10-phenanthroline)cobalt(II)</i>  | Zhong, Zeng & Luo (2006)             | 10.1107/S1600536806047295 | MEQFOE   |
| <i>Tris(quinolin-8-olato-κ<sup>2</sup>N,O)cobalt(III) glyoxal hemisolvate monohydrate</i>  | Zhong, Zeng, Liu & Luo (2006b)       | 10.1107/S1600536806050240 | MEQHEW   |
| <i>(8-Quinololinol-κ<sup>2</sup>N,O)bis(8-quinolinolato-κ<sup>2</sup>N,O)nickel(II) glyoxal hemisolvate monohydrate</i>  | Zhong, Zeng, Liu & Luo (2007)        | 10.1107/S1600536806053232 | METVUD   |
| <i>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate</i>   | Zhong, Zeng & Luo (2007)             | 10.1107/S1600536806053530 | METQIM   |
| <i>(8-Quinololinol-κ<sup>2</sup>N,O)-bis(8-quinolinolato-κ<sup>2</sup>N,O)zinc(II) glyoxal hemisolvate monohydrate</i>   | Zhong, Zeng, Luo, Li & Xiao (2007)   | 10.1107/S1600536807001171 | DEXTEG   |
| <i>(Dimethylglyoxime-κ<sup>2</sup>N,N')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')nickel(II) dinitrate dihydrate</i>  | Zhong, Zeng, Yang, Luo & Li (2007a)  | 10.1107/S1600536807004102 | YEYGOZ   |
| <i>(Dimethylglyoxime-κ<sup>2</sup>N,N')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')zinc(II) dinitrate dihydrate</i>  | Zhong, Zeng, Yang, Luo & Li (2007b)  | 10.1107/S1600536807004096 | YEYGUF   |
| <i>Chloridobis(1,10-phenanthroline-κN,N')copper(I) hexahydrate</i>   | Zhong, Zeng, Yang, Luo & Xiao (2007) | 10.1107/S160053680700791X | HEGKOU1  |
| <i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)</i>  | Zhong, Zeng, Yang & Luo (2007a)      | 10.1107/S1600536807017461 | ITCPCO1  |
| <i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)</i>  | Zhong, Zeng, Yang & Luo (2007b)      | 10.1107/S160053680701879X | AVUJEG02 |
| <i>Tetrakis(nitrato-κ<sup>2</sup>O,O')bis(4-phenylpyridine-κN)cerium(IV)</i>   | Zhong, Zeng, Yang & Luo (2007c)      | 10.1107/S1600536807018831 | CICDOI   |
| <i>Bis(4,4'-bipyridine-κ<sup>2</sup>N,N')tetrakis(nitrato-κ<sup>2</sup>O,O')cerium(IV)</i>   | Zhong, Zeng, Yang & Luo (2007d)      | 10.1107/S1600536807021502 | YIDNEF   |
| <i>(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)</i>   | Zhong, Zeng, Yang, Luo & Xu (2007)   | 10.1107/S1600536807027171 | EDUROL   |
| <i>(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)</i>  | Zhong, Yang, Luo & Xu (2007a)        | 10.1107/S1600536807028061 | EDUTUT   |
| <i>(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)</i>  | Zhong, Yang, Luo & Xu (2007b)        | 10.1107/S1600536807028693 | RIGQEE   |
| <i>(1,10-Phenanthroline-κ<sup>2</sup>N,N')tris(phenoxyacetato)-κO;κO;κO,O'-neodymium(III)</i>  | Zhong, Yang, Luo & Xu (2007c)        | 10.1107/S1600536807030371 | UDUMEM   |
| <i>Bis(2,2'-bipyridyl-κ<sup>2</sup>N,N')bis(thiocyanato-κN)nickel(II)</i>  | Zhong, Yang, Luo & Xu (2007d)        | 10.1107/S1600536807031613 | YEJGOJ01 |
| <i>Bis(2,2'-bipyridyl-κ<sup>2</sup>N,N')bis(isothiocyanato-κN)copper(II)</i>   | Zhong, Yang, Luo & Xu (2007e)        | 10.1107/S1600536807033181 | UFAPOH   |
| <i>Bis(2,2'-bipyridyl-κ<sup>2</sup>N,N')bis(thiocyanato-κN)zinc(II)</i>  | Zhong, Yang, Luo & Xu (2007f)        | 10.1107/S1600536807035337 | TIGFAR   |
| <i>(1,10-Phenanthroline-κ<sup>2</sup>N,N')tris(3-phenylpropanoato-κO)neodymium(III)</i>  | Zhong, Yang, Luo & Xu (2007g)        | 10.1107/S1600536807035350 | TIGFEV   |
| <i>2-Fluoro-3,5-dinitrobenzamide monohydrate</i>   | Zhong, Yang, Xie & Luo (2007j)       | 10.1107/S1600536807038676 | VIKGAY   |
| <i>2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)</i>  | Zhong, Yang, Xie & Luo (2007k)       | 10.1107/S1600536807039724 | KILKIA   |
| <i>1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate</i>   | Zhong, Yang, Xie & Luo (2007l)       | 10.1107/S1600536807040779 | AFETAH   |
| <i>N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)</i>  | Zhong, Yang, Xie & Luo (2007m)       | 10.1107/S160053680704086X | AFINAF   |
| <i>catena-Poly[[bis(μ-anilinoacetato-κ<sup>2</sup>O:O')bis(μ-anilinoacetato-κ<sup>2</sup>O:O')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')samarium(III)]-μ-anilinoacetato-κ<sup>2</sup>O:O']</i> | Zhong, Yang, Xie & Luo (2007a)       | 10.1107/S1600536807043528 | PILDAQ   |
| <i>2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate</i>  | Zhong, Yang, Xie & Luo (2007n)       | 10.1107/S1600536807045199 | XILWIZ   |
| <i>catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]</i>   | Zhong, Yang, Xie & Luo (2007b)       | 10.1107/S1600536807048489 | WIMWEV   |
| <i>Hexaaquacopper(II) bis(4-methylbenzenesulfonate)</i>  | Zhong, Yang, Xie & Luo (2007c)       | 10.1107/S1600536807049525 | TOLSCV01 |

**Table 1 (continued)**

| Title   | Reference                       | DOI                       | Refcode  |
|---|---------------------------------|---------------------------|----------|
| <i>catena-Poly[[tetra-<math>\mu</math>-anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di-<math>\mu</math>-anilinoacetato]</i>  | Zhong, Yang, Xie & Luo (2007d)  | 10.1107/S1600536807051240 | GIMZEI   |
| <i>Hexaaquachromium(II) bis(4-methylbenzenesulfonate)</i>   | Zhong, Yang, Xie & Luo (2007e)  | 10.1107/S1600536807051227 | GIMZIM   |
| <i>Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)</i>  | Zhong, Yang, Xie & Luo (2007f)  | 10.1107/S1600536807052051 | QUKQES01 |
| <i>catena-Poly[(acetato-<math>\kappa</math>O)(1,10-phenanthroline-<math>\kappa^2</math>N,N')cobalt(II)]-<math>\mu</math>-acetato-<math>\kappa^2</math>O:O']</i>   | Zhong, Yang, Xie & Luo (2007g)  | 10.1107/S1600536807053494 | NIQLAB   |
| <i>Hexaaquanickel(II) bis(4-aminobenzenesulfonate)</i>  | Zhong, Zhong, Xie & Luo (2007a) | 10.1107/S1600536807054372 | HIPZOW   |
| <i>catena-Poly[(acetato-<math>\kappa</math>O)(1,10-phenanthroline-<math>\kappa^2</math>N,N')copper(II)]-<math>\mu</math>-acetato-<math>\kappa^2</math>O:O']</i>   | Zhong, Yang, Xie & Luo (2007h)  | 10.1107/S160053680705622X | XIRGOV   |
| <i>Hexaaquazinc(II) bis(4-aminobenzenesulfonate)</i>  | Zhong, Zhong, Xie & Luo (2007b) | 10.1107/S1600536807056498 | XIRJEO   |
| <i>catena-Poly[(acetato-<math>\kappa</math>O)(1,10-phenanthroline-<math>\kappa^2</math>N,N')nickel(II)]-<math>\mu</math>-acetato-<math>\kappa^2</math>O:O']</i>   | Zhong, Yang, Xie & Luo (2007i)  | 10.1107/S1600536807058540 | HIQJOH   |
| <i>Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)</i>  | Zhong, Xie & Luo (2007)         | 10.1107/S1600536807058527 | HIQJUN   |
| <i>catena-Poly[[tetra-<math>\mu</math>-anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di-<math>\mu</math>-anilinoacetato]</i>   | Zhong, Yang, Duan & Hong (2007) | 10.1107/S1600536807060643 | YIQMAN   |
| <i>(Dimethylglyoxime-<math>\kappa^2</math>N,N')bis(1,10-phenanthroline-<math>\kappa^2</math>N,N')copper(II) dinitrate dihydrate</i>   | Zhong, Yang, Luo & Li (2007)    | 10.1107/S1600536807061193 | YIQNUI   |
| <i>catena-Poly[(1,10-phenanthroline-<math>\kappa^2</math>N,N')praseodymium(III)]-di-<math>\mu</math>-phenoxyacetato-<math>\kappa^4</math>O:O'-[(1,10-phenanthroline-<math>\kappa^2</math>N,N')praseodymium(III)]-di-<math>\mu</math>-phenoxyacetato-<math>\kappa^4</math>O:O'-di-<math>\mu</math>-phenoxyacetato-<math>\kappa^3</math>O,O':<math>\kappa^3</math>O:O,O']</i> | Zhong, Yang, Luo & Xu (2008)    | 10.1107/S1600536807068614 | GISJIC   |

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**catena-Poly[[tetra- $\mu$ -anilinoacetato-bis-(1,10-phenanthroline)dieuropium(III)]-di- $\mu$ -anilinoacetato]**

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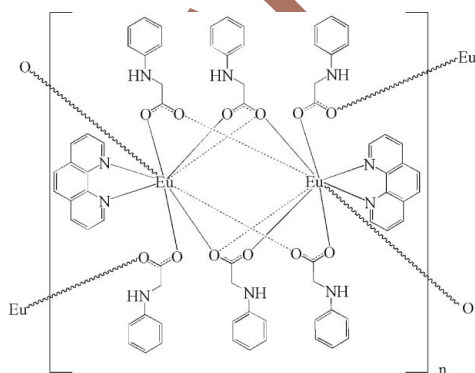
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Key indicators: single-crystal X-ray study;  $T = 273$  K; mean  $\sigma(\text{C}-\text{C}) = 0.012$  Å;  $R$  factor = 0.047;  $wR$  factor = 0.127; data-to-parameter ratio = 18.3.

In the crystal structure of the title compound,  $[\text{Eu}_2(\text{C}_8\text{H}_8\text{NO}_2)_6(\text{C}_{12}\text{H}_8\text{N}_2)_2]_n$ , the  $\text{Eu}^{\text{III}}$  atoms are bridged by two tridentate, two bidentate and four monodentate carboxylate groups with an inversion centre between the two  $\text{Eu}^{\text{III}}$  ions of this dinuclear structural unit. Each Eu atom is nine-coordinated by two 1,10-phenanthroline N atoms and seven O atoms of four anilinoacetate ligands. In the crystal structure, the chains are linked by  $\text{C}-\text{H}\cdots\text{N}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonds into a polymeric ribbon structure.

**Related literature**

For a related structure, see: Zhong *et al.* (2007a,b,c). For bond-length data, see: Allen *et al.* (1987).



**Experimental**

*Crystal data*

$[\text{Eu}_2(\text{C}_8\text{H}_8\text{NO}_2)_6(\text{C}_{12}\text{H}_8\text{N}_2)_2]$   
 $M_r = 1565.26$   
 Monoclinic,  $P2_1/n$   
 $a = 19.783$  (2) Å  
 $b = 8.8013$  (14) Å  
 $c = 21.2014$  (12) Å  
 $\beta = 105.816$  (5)°  
 $V = 3551.8$  (7) Å<sup>3</sup>

$Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.82$  mm<sup>-1</sup>

$T = 273$  (2) K  
 $0.34 \times 0.12 \times 0.09$  mm

*Data collection*

Bruker APEXII area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\text{min}} = 0.581$ ,  $T_{\text{max}} = 0.859$

27025 measured reflections  
 7520 independent reflections  
 4961 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.043$

*Refinement*

$R[F^2 > 2\sigma(F^2)] = 0.047$   
 $wR(F^2) = 0.127$   
 $S = 1.02$   
 7520 reflections  
 411 parameters  
 5 restraints

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 1.49$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.85$  e Å<sup>-3</sup>

**Table 1**  
 Selected geometric parameters (Å, °).

|                     |             |                      |             |
|---------------------|-------------|----------------------|-------------|
| Eu1—O1              | 2.608 (3)   | Eu1—O5 <sup>i</sup>  | 2.585 (3)   |
| Eu1—O2 <sup>i</sup> | 2.435 (3)   | Eu1—O6 <sup>ii</sup> | 2.576 (3)   |
| Eu1—O2              | 2.916 (4)   | Eu1—N1               | 2.700 (4)   |
| Eu1—O3              | 2.518 (3)   | Eu1—N2               | 2.776 (4)   |
| Eu1—O4              | 2.487 (3)   |                      |             |
| O1—Eu1—O2           | 47.12 (9)   | O2—Eu1—N1            | 102.55 (12) |
| O1—Eu1—O3           | 71.02 (11)  | O2—Eu1—N2            | 118.44 (11) |
| O1—Eu1—O4           | 140.70 (11) | O3—Eu1—N1            | 126.06 (12) |
| O2—Eu1—O3           | 64.84 (10)  | O3—Eu1—N2            | 79.59 (12)  |
| O2—Eu1—O4           | 139.91 (10) | O4—Eu1—N1            | 77.35 (12)  |
| O3—Eu1—O4           | 146.44 (11) | O4—Eu1—N2            | 96.70 (11)  |
| O1—Eu1—N1           | 65.09 (12)  | N1—Eu1—N2            | 60.42 (14)  |
| O1—Eu1—N2           | 75.12 (11)  |                      |             |

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

**Table 2**  
 Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$  | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{C}22-\text{H}22\text{B}\cdots\text{O}4^{\text{iii}}$ | 0.97         | 2.48               | 3.424 (7)   | 164                  |
| $\text{C}12-\text{H}12\cdots\text{N}4^{\text{ii}}$          | 0.93         | 2.53               | 3.380 (8)   | 151                  |
| $\text{C}12-\text{H}12\cdots\text{O}6^{\text{ii}}$          | 0.93         | 2.51               | 3.089 (7)   | 121                  |
| $\text{C}10-\text{H}10\cdots\text{O}1^{\text{iv}}$          | 0.93         | 2.45               | 3.314 (7)   | 154                  |
| $\text{C}1-\text{H}1\cdots\text{O}5^{\text{i}}$             | 0.93         | 2.41               | 3.121 (7)   | 134                  |

Symmetry codes: (i)  $-x + 2, -y, -z + 2$ ; (ii)  $-x + 2, -y + 1, -z + 2$ ; (iii)  $x, y - 1, z$ ; (iv)  $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{3}{2}$ .

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Siemens, 1996); 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: AT2497).

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Article retracted

**supplementary materials**

**Article retracted**

*Acta Cryst.* (2007). E63, m3142-m3143 [ doi:10.1107/S1600536807060643 ]

***catena*-Poly[[tetra- $\mu$ -anilinoacetato-bis(1,10-phenanthroline)dieuropium(III)]-di- $\mu$ -anilinoacetato]**

**H. Zhong, X.-M. Yang, S.-H. Duan and Y.-P. Hong**

### Comment

The crystal structure of  $[\text{RE}_2(\text{C}_8\text{H}_8\text{NO}_2)_6(\text{C}_{12}\text{H}_8\text{N}_2)_2]_n$  (RE = Sm, Nd and La), (II), have previously been reported (Zhong *et al.*, 2007a,b,c). The crystal structure determination of the title compound, (I), has been carried out in order to elucidate the molecular conformation and to compare it with that of (II). We report herein the crystal structure of (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The title compound,  $[\text{Eu}_2(\text{C}_8\text{H}_8\text{NO}_2)_6(\text{C}_{12}\text{H}_8\text{N}_2)_2]_n$ , which are bridged by two terdentate, two bidentate and four monodentate carboxyl groups with an inversion centre between the two  $\text{Eu}^{\text{III}}$  ions. Each Eu atom is nine-coordinated by two N atoms of 1,10-phenanthroline (phen) ligand and seven O atoms of four anilinoacetate ligands (Table 1). The Eu—O and Eu bonds are in the range of [2.435 (3)–2.916 (4) Å] and [2.700 (4) to 2.776 (4) Å], respectively, as in (II).

In the crystal structure, C—H $\cdots$ N and C—H $\cdots$ O hydrogen bonds (Fig. 2 and Table 2) seem to be effective in the stabilization of the structure, resulting in the formation of a supramolecular network structure, as in (II).

The four compounds, (I) and (II), are isostructural.

### Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Europium (III) nitrate hexahydrate (206.7 mg, 0.5 mmol), phen (198 mg, 1 mmol), anilinoacetic acid (292.4 mg, 2 mmol), ammonia (0.5 mol/l, 4 ml) and distilled water (8 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 453 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colorless solution was decanted from small colorless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

### Refinement

H3A and H4A (for NH) were located in difference syntheses and refined isotropically [N—H = 0.78 (3) and 0.83 (6) Å,  $U_{\text{iso}}(\text{H}) = 0.07$  (1) and 0.08 (2) Å<sup>2</sup>]. The H atoms were positioned geometrically, with N—H = 0.86 Å (for NH) and C—H = 0.93–0.97 Å (for CH), and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C}, \text{N})$ , where  $x = 1.2$  for aromatic and NH H atoms and  $x = 1.5$  for methyl H atoms.

Figures

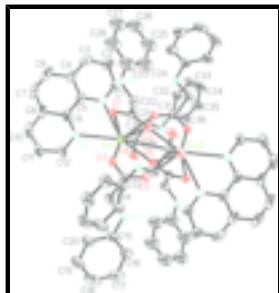


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level [symmetry code (A):  $2 - x, -y, 2 - z$ ]. All H atoms have been omitted for clarity.

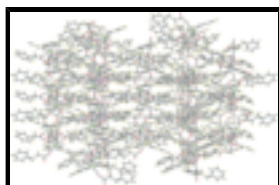


Fig. 2. A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

**catena-Poly[[tetra- $\mu$ -anilinoacetato-bis(1,10-phenanthroline)dieuropium(III)]-di- $\mu$ -anilinoacetato]**

*Crystal data*

[Eu<sub>2</sub>(C<sub>8</sub>H<sub>8</sub>NO<sub>2</sub>)<sub>6</sub>(C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>)<sub>2</sub>]

$M_r = 1565.26$

Monoclinic,  $P2_1/n$

Hall symbol:  $-P\ 2_1n$

$a = 19.783\ (2)\ \text{\AA}$

$b = 8.8013\ (14)\ \text{\AA}$

$c = 21.2014\ (12)\ \text{\AA}$

$\beta = 105.816\ (5)^\circ$

$V = 3551.8\ (7)\ \text{\AA}^3$

$Z = 2$

$F_{000} = 1576$

$D_x = 1.464\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073\ \text{\AA}$

Cell parameters from 9044 reflections

$\theta = 2.7\text{--}26.1^\circ$

$\mu = 1.82\ \text{mm}^{-1}$

$T = 273\ (2)\ \text{K}$

Plane, colourless

$0.34 \times 0.12 \times 0.09\ \text{mm}$

*Data collection*

Bruker APEXII area-detector  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273\ (2)\ \text{K}$

$\varphi$  and  $\omega$  scans

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

$T_{\min} = 0.581, T_{\max} = 0.859$

27025 measured reflections

7520 independent reflections

4961 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.043$

$\theta_{\text{max}} = 27.0^\circ$

$\theta_{\text{min}} = 2.0^\circ$

$h = -25 \rightarrow 24$

$k = -10 \rightarrow 11$

$l = -26 \rightarrow 26$

Refinement

|  |  |
|--|--|
| Refinement on $F^2$  | Secondary atom site location: difference Fourier map                   |
| Least-squares matrix: full                                     | Hydrogen site location: inferred from neighbouring sites               |
| $R[F^2 > 2\sigma(F^2)] = 0.047$                                | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.127$  | $w = 1/[\sigma^2(F_o^2) + (0.0708P)^2 + 1.1179P]$                      |
| $S = 1.02$   | where $P = (F_o^2 + 2F_c^2)/3$   |
| 7520 reflections   | $(\Delta/\sigma)_{\max} = 0.002$                                       |
| 411 parameters   | $\Delta\rho_{\max} = 1.49 \text{ e } \text{\AA}^{-3}$                  |
| 5 restraints   | $\Delta\rho_{\min} = -0.85 \text{ e } \text{\AA}^{-3}$                 |
| Primary atom site location: structure-invariant direct methods | 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 ( $\text{\AA}^2$ )

|     | $x$           | $y$         | $z$           | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|---------------|-------------|---------------|----------------------------------|
| Eu1 | 0.931209 (13) | 0.19067 (3) | 0.964289 (11) | 0.04106 (11)                     |
| O1  | 0.84657 (16)  | -0.0352 (4) | 0.91894 (16)  | 0.0422 (8)                       |
| O2  | 0.94691 (17)  | -0.1382 (4) | 0.97736 (16)  | 0.0476 (8)                       |
| O3  | 0.97044 (17)  | 0.0609 (4)  | 0.87446 (15)  | 0.0452 (8)                       |
| O4  | 0.93985 (18)  | 0.4212 (4)  | 1.03389 (15)  | 0.0448 (8)                       |
| O5  | 1.06684 (18)  | -0.0828 (4) | 0.92183 (16)  | 0.0473 (8)                       |
| O6  | 1.0076 (2)    | 0.6122 (4)  | 1.09116 (16)  | 0.0539 (9)                       |
| N1  | 0.7970 (2)    | 0.2338 (5)  | 0.9672 (2)    | 0.0455 (10)                      |
| N2  | 0.8341 (2)    | 0.3067 (4)  | 0.8547 (2)    | 0.0468 (10)                      |
| N3  | 1.1191 (2)    | -0.0134 (6) | 0.8228 (2)    | 0.0469 (11)                      |
| N5  | 0.7853 (2)    | -0.3271 (4) | 0.8984 (2)    | 0.0450 (10)                      |
| H5A | 0.7628        | -0.3417     | 0.8580        | 0.054*                           |
| N4  | 0.9877 (2)    | 0.5262 (5)  | 1.20640 (19)  | 0.0436 (10)                      |
| C1  | 0.7784 (3)    | 0.1908 (7)  | 1.0196 (3)    | 0.0620 (16)                      |
| H1  | 0.8133        | 0.1671      | 1.0576        | 0.074*                           |
| C2  | 0.7090 (3)    | 0.1799 (9)  | 1.0198 (4)    | 0.083 (2)                        |



## supplementary materials

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|      |            |              |            |             |
|------|------------|--------------|------------|-------------|
| H2   | 0.6964     | 0.1530       | 1.0575     | 0.100*      |
| C3   | 0.6584 (4) | 0.2107 (9)   | 0.9612 (5) | 0.092 (3)   |
| H3   | 0.6113     | 0.1982       | 0.9599     | 0.110*      |
| C4   | 0.6742 (3) | 0.2585 (9)   | 0.9055 (4) | 0.077 (2)   |
| C5   | 0.7465 (3) | 0.2678 (6)   | 0.9087 (3) | 0.0507 (13) |
| C6   | 0.6224 (4) | 0.2954 (11)  | 0.8388 (5) | 0.109 (3)   |
| H6   | 0.5746     | 0.2829       | 0.8343     | 0.131*      |
| C7   | 0.6419 (4) | 0.3435 (10)  | 0.7880 (4) | 0.100 (3)   |
| H7   | 0.6081     | 0.3710       | 0.7498     | 0.120*      |
| C8   | 0.7132 (3) | 0.3537 (8)   | 0.7907 (3) | 0.0671 (18) |
| C9   | 0.7661 (3) | 0.3098 (6)   | 0.8509 (3) | 0.0499 (13) |
| C10  | 0.7359 (5) | 0.4045 (8)   | 0.7374 (3) | 0.087 (2)   |
| H10  | 0.7036     | 0.4400       | 0.6998     | 0.104*      |
| C11  | 0.8044 (5) | 0.4017 (8)   | 0.7407 (3) | 0.080 (2)   |
| H11  | 0.8203     | 0.4321       | 0.7053     | 0.096*      |
| C12  | 0.8528 (3) | 0.3502 (7)   | 0.8007 (3) | 0.0610 (15) |
| H12  | 0.9002     | 0.3468       | 0.8024     | 0.073*      |
| C13  | 1.0285 (3) | 0.0026 (6)   | 0.8770 (2) | 0.0409 (11) |
| C14  | 1.0524 (3) | 0.0510 (7)   | 0.8173 (3) | 0.0512 (13) |
| H14A | 1.0191     | 0.0160       | 0.7775     | 0.061*      |
| H14B | 1.0552     | 0.1609       | 0.8156     | 0.061*      |
| C15  | 1.1463 (3) | 0.0138 (7)   | 0.7702 (3) | 0.0610 (15) |
| C16  | 1.2071 (3) | -0.0572 (9)  | 0.7757 (3) | 0.0765 (19) |
| H16  | 1.2269     | -0.1189      | 0.8116     | 0.092*      |
| C17  | 1.2400 (4) | -0.0367 (10) | 0.7266 (5) | 0.093 (2)   |
| H17  | 1.2830     | -0.0833      | 0.7301     | 0.111*      |
| C18  | 1.2100 (5) | 0.0521 (10)  | 0.6723 (5) | 0.106 (3)   |
| H18  | 1.2330     | 0.0624       | 0.6397     | 0.128*      |
| C19  | 1.1477 (5) | 0.1245 (11)  | 0.6655 (4) | 0.109 (3)   |
| H19  | 1.1278     | 0.1841       | 0.6289     | 0.131*      |
| C20  | 1.1147 (4) | 0.1063 (9)   | 0.7152 (4) | 0.083 (2)   |
| H20  | 1.0722     | 0.1546       | 0.7124     | 0.100*      |
| C21  | 0.8840 (3) | -0.1515 (6)  | 0.9389 (2) | 0.0431 (12) |
| C22  | 0.8583 (3) | -0.3150 (6)  | 0.9197 (3) | 0.0545 (14) |
| H22A | 0.8780     | -0.3501      | 0.8852     | 0.065*      |
| H22B | 0.8756     | -0.3809      | 0.9573     | 0.065*      |
| C23  | 0.7535 (7) | -0.3143 (10) | 0.9462 (7) | 0.1243 (16) |
| C24  | 0.7846 (6) | -0.2767 (10) | 1.0124 (7) | 0.1243 (16) |
| H24  | 0.8326     | -0.2584      | 1.0277     | 0.149*      |
| C25  | 0.7421 (6) | -0.2681 (11) | 1.0536 (7) | 0.1243 (16) |
| H25  | 0.7602     | -0.2451      | 1.0978     | 0.149*      |
| C26  | 0.6719 (6) | -0.2946 (10) | 1.0268 (7) | 0.1243 (16) |
| H26  | 0.6431     | -0.2843      | 1.0547     | 0.149*      |
| C27  | 0.6385 (6) | -0.3358 (10) | 0.9615 (6) | 0.1243 (16) |
| H27  | 0.5908     | -0.3579      | 0.9476     | 0.149*      |
| C28  | 0.6802 (6) | -0.3414 (10) | 0.9198 (6) | 0.1243 (16) |
| H28  | 0.6613     | -0.3623      | 0.8755     | 0.149*      |
| C29  | 0.9697 (3) | 0.4996 (6)   | 1.0863 (2) | 0.0417 (11) |
| C30  | 0.9484 (3) | 0.4461 (7)   | 1.1474 (2) | 0.0542 (14) |

|      |             |             |             |             |
|------|-------------|-------------|-------------|-------------|
| H30A | 0.8986      | 0.4634      | 1.1408      | 0.065*      |
| H30B | 0.9570      | 0.3378      | 1.1533      | 0.065*      |
| C31  | 0.9743 (3)  | 0.4892 (6)  | 1.2657 (2)  | 0.0521 (13) |
| C32  | 0.9280 (3)  | 0.3784 (9)  | 1.2720 (3)  | 0.0706 (18) |
| H32  | 0.9027      | 0.3236      | 1.2357      | 0.085*      |
| C33  | 0.9196 (5)  | 0.3497 (12) | 1.3341 (4)  | 0.109 (3)   |
| H33  | 0.8893      | 0.2730      | 1.3393      | 0.130*      |
| C34  | 0.9573 (5)  | 0.4368 (12) | 1.3906 (3)  | 0.102 (3)   |
| H34  | 0.9497      | 0.4196      | 1.4314      | 0.122*      |
| C35  | 1.0033 (4)  | 0.5429 (9)  | 1.3832 (3)  | 0.086 (2)   |
| H35  | 1.0284      | 0.5984      | 1.4193      | 0.103*      |
| C36  | 1.0139 (3)  | 0.5704 (8)  | 1.3220 (3)  | 0.0705 (17) |
| H36  | 1.0470      | 0.6420      | 1.3177      | 0.085*      |
| H4A  | 0.959 (3)   | 0.596 (6)   | 1.204 (3)   | 0.08 (2)*   |
| H3A  | 1.1044 (17) | -0.091 (3)  | 0.8091 (16) | 0.07 (1)*   |

Atomic displacement parameters ( $\text{\AA}^2$ )

|     | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$      | $U^{13}$     | $U^{23}$     |
|-----|--------------|--------------|--------------|---------------|--------------|--------------|
| Eu1 | 0.04517 (16) | 0.03736 (17) | 0.03679 (15) | -0.00155 (12) | 0.00464 (10) | 0.00065 (11) |
| O1  | 0.0382 (17)  | 0.0343 (19)  | 0.0479 (19)  | 0.0005 (15)   | 0.0008 (14)  | -0.0027 (15) |
| O2  | 0.0393 (18)  | 0.051 (2)    | 0.045 (2)    | -0.0022 (16)  | 0.0000 (15)  | 0.0083 (16)  |
| O3  | 0.050 (2)    | 0.049 (2)    | 0.0379 (18)  | 0.0054 (17)   | 0.0138 (15)  | 0.0020 (16)  |
| O4  | 0.061 (2)    | 0.0342 (19)  | 0.0396 (18)  | -0.0046 (16)  | 0.0139 (15)  | -0.0048 (15) |
| O5  | 0.055 (2)    | 0.049 (2)    | 0.0406 (19)  | 0.0089 (17)   | 0.0176 (16)  | 0.0107 (16)  |
| O6  | 0.074 (2)    | 0.050 (2)    | 0.039 (2)    | -0.025 (2)    | 0.0186 (17)  | -0.0034 (16) |
| N1  | 0.042 (2)    | 0.040 (2)    | 0.049 (3)    | 0.0031 (19)   | 0.0033 (19)  | -0.0093 (19) |
| N2  | 0.057 (3)    | 0.039 (2)    | 0.036 (2)    | 0.003 (2)     | -0.0015 (18) | 0.0002 (18)  |
| N3  | 0.047 (2)    | 0.054 (3)    | 0.045 (3)    | 0.006 (2)     | 0.022 (2)    | 0.010 (2)    |
| N5  | 0.037 (2)    | 0.032 (2)    | 0.056 (3)    | -0.0128 (17)  | -0.0045 (18) | -0.0075 (18) |
| N4  | 0.061 (3)    | 0.043 (3)    | 0.028 (2)    | -0.021 (2)    | 0.0151 (19)  | -0.0060 (18) |
| C1  | 0.051 (3)    | 0.077 (5)    | 0.058 (4)    | 0.008 (3)     | 0.015 (3)    | -0.002 (3)   |
| C2  | 0.051 (4)    | 0.116 (7)    | 0.087 (5)    | 0.005 (4)     | 0.027 (4)    | -0.010 (4)   |
| C3  | 0.043 (4)    | 0.109 (7)    | 0.122 (7)    | -0.006 (4)    | 0.020 (4)    | -0.014 (5)   |
| C4  | 0.046 (3)    | 0.085 (5)    | 0.083 (5)    | 0.008 (3)     | -0.009 (3)   | -0.021 (4)   |
| C5  | 0.048 (3)    | 0.035 (3)    | 0.062 (4)    | 0.007 (2)     | 0.002 (3)    | -0.011 (2)   |
| C6  | 0.049 (4)    | 0.146 (9)    | 0.107 (7)    | 0.017 (5)     | -0.021 (4)   | -0.027 (6)   |
| C7  | 0.075 (5)    | 0.115 (7)    | 0.078 (5)    | 0.039 (5)     | -0.031 (4)   | -0.015 (5)   |
| C8  | 0.067 (4)    | 0.068 (4)    | 0.046 (4)    | 0.018 (3)     | -0.018 (3)   | -0.010 (3)   |
| C9  | 0.054 (3)    | 0.033 (3)    | 0.050 (3)    | 0.006 (2)     | -0.009 (2)   | -0.003 (2)   |
| C10 | 0.113 (6)    | 0.070 (5)    | 0.050 (4)    | 0.018 (4)     | -0.024 (4)   | -0.001 (3)   |
| C11 | 0.116 (6)    | 0.074 (5)    | 0.038 (3)    | -0.002 (4)    | 0.002 (3)    | 0.009 (3)    |
| C12 | 0.075 (4)    | 0.055 (4)    | 0.046 (3)    | -0.002 (3)    | 0.004 (3)    | 0.010 (3)    |
| C13 | 0.050 (3)    | 0.034 (3)    | 0.038 (3)    | -0.008 (2)    | 0.011 (2)    | -0.004 (2)   |
| C14 | 0.060 (3)    | 0.051 (3)    | 0.045 (3)    | 0.007 (3)     | 0.018 (2)    | 0.011 (2)    |
| C15 | 0.064 (4)    | 0.069 (4)    | 0.057 (4)    | -0.009 (3)    | 0.029 (3)    | 0.000 (3)    |
| C16 | 0.072 (4)    | 0.094 (5)    | 0.074 (4)    | 0.005 (4)     | 0.037 (4)    | 0.001 (4)    |
| C17 | 0.082 (5)    | 0.097 (6)    | 0.117 (6)    | -0.008 (5)    | 0.057 (5)    | -0.010 (5)   |

## supplementary materials

|     |           |           |           |            |           |            |
|-----|-----------|-----------|-----------|------------|-----------|------------|
| C18 | 0.138 (8) | 0.085 (6) | 0.133 (8) | -0.018 (6) | 0.101 (7) | -0.001 (6) |
| C19 | 0.148 (8) | 0.115 (7) | 0.092 (6) | 0.021 (6)  | 0.078 (6) | 0.035 (5)  |
| C20 | 0.096 (5) | 0.089 (5) | 0.082 (5) | 0.004 (4)  | 0.056 (4) | 0.023 (4)  |
| C21 | 0.043 (3) | 0.052 (3) | 0.031 (2) | -0.007 (2) | 0.004 (2) | -0.005 (2) |
| C22 | 0.057 (3) | 0.043 (3) | 0.059 (3) | 0.003 (3)  | 0.007 (3) | -0.008 (3) |
| C23 | 0.132 (4) | 0.090 (3) | 0.174 (5) | 0.015 (3)  | 0.082 (4) | 0.031 (3)  |
| C24 | 0.132 (4) | 0.090 (3) | 0.174 (5) | 0.015 (3)  | 0.082 (4) | 0.031 (3)  |
| C25 | 0.132 (4) | 0.090 (3) | 0.174 (5) | 0.015 (3)  | 0.082 (4) | 0.031 (3)  |
| C26 | 0.132 (4) | 0.090 (3) | 0.174 (5) | 0.015 (3)  | 0.082 (4) | 0.031 (3)  |
| C27 | 0.132 (4) | 0.090 (3) | 0.174 (5) | 0.015 (3)  | 0.082 (4) | 0.031 (3)  |
| C28 | 0.132 (4) | 0.090 (3) | 0.174 (5) | 0.015 (3)  | 0.082 (4) | 0.031 (3)  |
| C29 | 0.055 (3) | 0.032 (3) | 0.039 (3) | -0.001 (2) | 0.013 (2) | 0.004 (2)  |
| C30 | 0.070 (3) | 0.054 (3) | 0.040 (3) | -0.021 (3) | 0.017 (2) | -0.007 (2) |
| C31 | 0.068 (3) | 0.054 (3) | 0.034 (3) | -0.002 (3) | 0.014 (2) | 0.004 (2)  |
| C32 | 0.071 (4) | 0.094 (5) | 0.049 (3) | -0.031 (4) | 0.020 (3) | -0.002 (3) |
| C33 | 0.122 (7) | 0.142 (8) | 0.078 (5) | -0.050 (6) | 0.053 (5) | 0.001 (5)  |
| C34 | 0.114 (6) | 0.151 (8) | 0.047 (4) | -0.030 (6) | 0.035 (4) | 0.003 (5)  |
| C35 | 0.106 (5) | 0.106 (6) | 0.041 (3) | -0.021 (5) | 0.013 (3) | -0.010 (4) |
| C36 | 0.082 (4) | 0.075 (5) | 0.051 (3) | -0.019 (4) | 0.013 (3) | -0.010 (3) |

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

|                      |            |          |            |
|----------------------|------------|----------|------------|
| Eu1—O1               | 2.608 (3)  | C10—C11  | 1.337 (10) |
| Eu1—O2 <sup>i</sup>  | 2.435 (3)  | C10—H10  | 0.9300     |
| Eu1—O2               | 2.916 (4)  | C11—C12  | 1.441 (8)  |
| Eu1—O3               | 2.518 (3)  | C11—H11  | 0.9300     |
| Eu1—O4               | 2.487 (3)  | C12—H12  | 0.9300     |
| Eu1—O5 <sup>i</sup>  | 2.585 (3)  | C13—C14  | 1.528 (7)  |
| Eu1—O6 <sup>ii</sup> | 2.576 (3)  | C14—H14A | 0.9700     |
| Eu1—N1               | 2.700 (4)  | C14—H14B | 0.9700     |
| Eu1—N2               | 2.776 (4)  | C15—C16  | 1.332 (9)  |
| Eu1—Eu1 <sup>i</sup> | 4.3265 (7) | C15—C20  | 1.420 (9)  |
| O1—C21               | 1.267 (6)  | C16—C17  | 1.382 (10) |
| O2—C21               | 1.293 (6)  | C16—H16  | 0.9300     |
| O2—Eu1 <sup>i</sup>  | 2.435 (3)  | C17—C18  | 1.384 (12) |
| O3—C13               | 1.245 (6)  | C17—H17  | 0.9300     |
| O4—C29               | 1.304 (6)  | C18—C19  | 1.361 (12) |
| O5—C13               | 1.284 (6)  | C18—H18  | 0.9300     |
| O5—Eu1 <sup>i</sup>  | 2.585 (3)  | C19—C20  | 1.391 (9)  |
| O6—C29               | 1.230 (6)  | C19—H19  | 0.9300     |
| O6—Eu1 <sup>ii</sup> | 2.576 (3)  | C20—H20  | 0.9300     |
| N1—C1                | 1.317 (7)  | C21—C22  | 1.544 (7)  |
| N1—C5                | 1.395 (7)  | C22—H22A | 0.9700     |
| N2—C9                | 1.325 (7)  | C22—H22B | 0.9700     |
| N2—C12               | 1.350 (7)  | C23—C24  | 1.410 (17) |
| N3—C15               | 1.386 (7)  | C23—C28  | 1.426 (16) |
| N3—C14               | 1.411 (6)  | C24—C25  | 1.368 (14) |
| N3—H3A               | 0.78 (3)   | C24—H24  | 0.9300     |

|                                       |             |               |            |
|---------------------------------------|-------------|---------------|------------|
| N5—C23                                | 1.337 (12)  | C25—C26       | 1.371 (16) |
| N5—C22                                | 1.393 (7)   | C25—H25       | 0.9300     |
| N5—H5A                                | 0.8600      | C26—C27       | 1.410 (16) |
| N4—C31                                | 1.392 (6)   | C26—H26       | 0.9300     |
| N4—C30                                | 1.461 (6)   | C27—C28       | 1.364 (13) |
| N4—H4A                                | 0.83 (6)    | C27—H27       | 0.9300     |
| C1—C2                                 | 1.379 (9)   | C28—H28       | 0.9300     |
| C1—H1                                 | 0.9300      | C29—C30       | 1.541 (7)  |
| C2—C3                                 | 1.393 (12)  | C30—H30A      | 0.9700     |
| C2—H2                                 | 0.9300      | C30—H30B      | 0.9700     |
| C3—C4                                 | 1.369 (12)  | C31—C32       | 1.369 (8)  |
| C3—H3                                 | 0.9300      | C31—C36       | 1.428 (8)  |
| C4—C5                                 | 1.414 (9)   | C32—C33       | 1.394 (9)  |
| C4—C6                                 | 1.538 (11)  | C32—H32       | 0.9300     |
| C5—C9                                 | 1.431 (8)   | C33—C34       | 1.445 (11) |
| C6—C7                                 | 1.309 (13)  | C33—H33       | 0.9300     |
| C6—H6                                 | 0.9300      | C34—C35       | 1.344 (10) |
| C7—C8                                 | 1.398 (11)  | C34—H34       | 0.9300     |
| C7—H7                                 | 0.9300      | C35—C36       | 1.390 (9)  |
| C8—C10                                | 1.399 (10)  | C35—H35       | 0.9300     |
| C8—C9                                 | 1.466 (7)   | C36—H36       | 0.9300     |
| O1—Eu1—O2                             | 47.12 (9)   | C5—C9—C8      | 121.2 (5)  |
| O1—Eu1—O3                             | 71.02 (11)  | C11—C10—C8    | 119.7 (6)  |
| O1—Eu1—O4                             | 140.70 (11) | C11—C10—H10   | 120.1      |
| O2—Eu1—O3                             | 64.84 (10)  | C8—C10—H10    | 120.1      |
| O2—Eu1—O4                             | 139.91 (10) | C10—C11—C12   | 118.2 (7)  |
| O3—Eu1—O4                             | 146.44 (11) | C10—C11—H11   | 120.9      |
| O1—Eu1—N1                             | 65.09 (12)  | C12—C11—H11   | 120.9      |
| O1—Eu1—N2                             | 75.12 (11)  | N2—C12—C11    | 124.6 (6)  |
| O2—Eu1—N1                             | 102.55 (12) | N2—C12—H12    | 117.7      |
| O2—Eu1—N2                             | 118.44 (11) | C11—C12—H12   | 117.7      |
| O3—Eu1—N1                             | 126.06 (12) | O3—C13—O5     | 128.7 (4)  |
| O3—Eu1—N2                             | 79.59 (12)  | O3—C13—C14    | 109.8 (4)  |
| O4—Eu1—N1                             | 77.35 (12)  | O5—C13—C14    | 121.4 (4)  |
| O4—Eu1—N2                             | 96.70 (11)  | N3—C14—C13    | 108.3 (4)  |
| N1—Eu1—N2                             | 60.42 (14)  | N3—C14—H14A   | 110.0      |
| O2 <sup>i</sup> —Eu1—O4               | 87.41 (12)  | C13—C14—H14A  | 110.0      |
| O2 <sup>i</sup> —Eu1—O3               | 80.31 (11)  | N3—C14—H14B   | 110.0      |
| O2 <sup>i</sup> —Eu1—O6 <sup>ii</sup> | 80.57 (12)  | C13—C14—H14B  | 110.0      |
| O4—Eu1—O6 <sup>ii</sup>               | 75.90 (11)  | H14A—C14—H14B | 108.4      |
| O3—Eu1—O6 <sup>ii</sup>               | 71.35 (11)  | C16—C15—N3    | 112.8 (6)  |
| O2 <sup>i</sup> —Eu1—O5 <sup>i</sup>  | 72.25 (11)  | C16—C15—C20   | 121.8 (6)  |
| O4—Eu1—O5 <sup>i</sup>                | 76.37 (11)  | N3—C15—C20    | 125.4 (6)  |
| O3—Eu1—O5 <sup>i</sup>                | 127.64 (11) | C15—C16—C17   | 118.1 (7)  |
| O6 <sup>ii</sup> —Eu1—O5 <sup>i</sup> | 141.68 (11) | C15—C16—H16   | 120.9      |
| O2 <sup>i</sup> —Eu1—O1               | 119.34 (12) | C17—C16—H16   | 120.9      |

## supplementary materials

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|  |             |               |            |
|--|-------------|---------------|------------|
| O6 <sup>ii</sup> —Eu1—O1               | 132.82 (11) | C16—C17—C18   | 121.2 (7)  |
| O5 <sup>i</sup> —Eu1—O1                | 84.78 (11)  | C16—C17—H17   | 119.4      |
| O2 <sup>i</sup> —Eu1—N1                | 149.20 (12) | C18—C17—H17   | 119.4      |
| O6 <sup>ii</sup> —Eu1—N1               | 120.21 (14) | C19—C18—C17   | 121.5 (7)  |
| O5 <sup>i</sup> —Eu1—N1                | 78.16 (12)  | C19—C18—H18   | 119.2      |
| O2 <sup>i</sup> —Eu1—N2                | 149.19 (13) | C17—C18—H18   | 119.2      |
| O6 <sup>ii</sup> —Eu1—N2               | 70.99 (13)  | C18—C19—C20   | 117.6 (8)  |
| O5 <sup>i</sup> —Eu1—N2                | 138.42 (12) | C18—C19—H19   | 121.2      |
| O2 <sup>i</sup> —Eu1—O2                | 72.45 (13)  | C20—C19—H19   | 121.2      |
| O6 <sup>ii</sup> —Eu1—O2               | 131.37 (11) | C19—C20—C15   | 119.7 (7)  |
| O5 <sup>i</sup> —Eu1—O2                | 64.69 (10)  | C19—C20—H20   | 120.1      |
| O2 <sup>i</sup> —Eu1—Eu1 <sup>i</sup>  | 39.99 (9)   | C15—C20—H20   | 120.1      |
| O4—Eu1—Eu1 <sup>i</sup>                | 119.35 (8)  | O1—C21—O2     | 120.8 (5)  |
| O3—Eu1—Eu1 <sup>i</sup>                | 67.59 (8)   | O1—C21—C22    | 122.9 (4)  |
| O6 <sup>ii</sup> —Eu1—Eu1 <sup>i</sup> | 110.69 (9)  | O2—C21—C22    | 116.3 (5)  |
| O5 <sup>i</sup> —Eu1—Eu1 <sup>i</sup>  | 62.63 (7)   | N5—C22—C21    | 113.3 (4)  |
| O1—Eu1—Eu1 <sup>i</sup>                | 79.46 (7)   | N5—C22—H22A   | 108.9      |
| N1—Eu1—Eu1 <sup>i</sup>                | 129.05 (10) | C21—C22—H22A  | 108.9      |
| N2—Eu1—Eu1 <sup>i</sup>                | 143.56 (8)  | N5—C22—H22B   | 108.9      |
| O2—Eu1—Eu1 <sup>i</sup>                | 32.46 (6)   | C21—C22—H22B  | 108.9      |
| C21—O1—Eu1                             | 103.5 (3)   | H22A—C22—H22B | 107.7      |
| C21—O2—Eu1 <sup>i</sup>                | 162.2 (4)   | N5—C23—C24    | 127.4 (11) |
| C21—O2—Eu1                             | 88.3 (3)    | N5—C23—C28    | 109.1 (12) |
| Eu1 <sup>i</sup> —O2—Eu1               | 107.55 (13) | C24—C23—C28   | 123.5 (11) |
| C13—O3—Eu1                             | 128.7 (3)   | C25—C24—C23   | 118.1 (12) |
| C29—O4—Eu1                             | 151.5 (3)   | C25—C24—H24   | 121.0      |
| C13—O5—Eu1 <sup>i</sup>                | 139.5 (3)   | C23—C24—H24   | 121.0      |
| C29—O6—Eu1 <sup>ii</sup>               | 148.9 (3)   | C24—C25—C26   | 117.2 (13) |
| C1—N1—C5                               | 120.9 (5)   | C24—C25—H25   | 121.4      |
| C1—N1—Eu1                              | 118.7 (4)   | C26—C25—H25   | 121.4      |
| C5—N1—Eu1                              | 118.7 (3)   | C25—C26—C27   | 126.9 (11) |
| C9—N2—C12                              | 116.9 (5)   | C25—C26—H26   | 116.5      |
| C9—N2—Eu1                              | 121.1 (3)   | C27—C26—H26   | 116.5      |
| C12—N2—Eu1                             | 121.8 (4)   | C28—C27—C26   | 116.2 (12) |
| C15—N3—C14                             | 115.1 (4)   | C28—C27—H27   | 121.9      |
| C15—N3—H3A                             | 92 (3)      | C26—C27—H27   | 121.9      |
| C14—N3—H3A                             | 95 (3)      | C27—C28—C23   | 118.0 (13) |
| C23—N5—C22                             | 114.0 (7)   | C27—C28—H28   | 121.0      |
| C23—N5—H5A                             | 123.0       | C23—C28—H28   | 121.0      |
| C22—N5—H5A                             | 123.0       | O6—C29—O4     | 128.5 (4)  |
| C31—N4—C30                             | 118.2 (4)   | O6—C29—C30    | 118.4 (4)  |
| C31—N4—H4A                             | 86 (5)      | O4—C29—C30    | 113.0 (4)  |
| C30—N4—H4A                             | 96 (5)      | N4—C30—C29    | 111.7 (4)  |
| N1—C1—C2                               | 122.0 (6)   | N4—C30—H30A   | 109.3      |

|           |           |               |           |
|-----------|-----------|---------------|-----------|
| N1—C1—H1  | 119.0     | C29—C30—H30A  | 109.3     |
| C2—C1—H1  | 119.0     | N4—C30—H30B   | 109.3     |
| C1—C2—C3  | 117.2 (7) | C29—C30—H30B  | 109.3     |
| C1—C2—H2  | 121.4     | H30A—C30—H30B | 107.9     |
| C3—C2—H2  | 121.4     | C32—C31—N4    | 123.5 (5) |
| C4—C3—C2  | 123.5 (6) | C32—C31—C36   | 120.3 (5) |
| C4—C3—H3  | 118.3     | N4—C31—C36    | 116.2 (5) |
| C2—C3—H3  | 118.3     | C32—C31—H4A   | 122 (3)   |
| C3—C4—C5  | 116.2 (6) | C36—C31—H4A   | 109 (2)   |
| C3—C4—C6  | 127.3 (7) | C31—C32—C33   | 118.4 (6) |
| C5—C4—C6  | 116.4 (8) | C31—C32—H32   | 120.8     |
| N1—C5—C4  | 120.0 (6) | C33—C32—H32   | 120.8     |
| N1—C5—C9  | 121.3 (5) | C32—C33—C34   | 121.3 (7) |
| C4—C5—C9  | 118.6 (6) | C32—C33—H33   | 119.4     |
| C7—C6—C4  | 123.5 (8) | C34—C33—H33   | 119.4     |
| C7—C6—H6  | 118.2     | C35—C34—C33   | 119.0 (6) |
| C4—C6—H6  | 118.2     | C35—C34—H34   | 120.5     |
| C6—C7—C8  | 120.5 (7) | C33—C34—H34   | 120.5     |
| C6—C7—H7  | 119.8     | C34—C35—C36   | 120.6 (7) |
| C8—C7—H7  | 119.8     | C34—C35—H35   | 119.7     |
| C7—C8—C10 | 122.0 (7) | C36—C35—H35   | 119.7     |
| C7—C8—C9  | 119.5 (7) | C35—C36—C31   | 120.3 (6) |
| C10—C8—C9 | 118.5 (6) | C35—C36—H36   | 119.8     |
| N2—C9—C5  | 116.8 (4) | C31—C36—H36   | 119.8     |
| N2—C9—C8  | 122.0 (6) |               |           |

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

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

| <i>D</i> —H... <i>A</i>      | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|------------------------------|-------------|---------------|-----------------------|-------------------------|
| C22—H22B...O4 <sup>iii</sup> | 0.97        | 2.48          | 3.424 (7)             | 164                     |
| C12—H12...N4 <sup>ii</sup>   | 0.93        | 2.53          | 3.380 (8)             | 151                     |
| C12—H12...O6 <sup>ii</sup>   | 0.93        | 2.51          | 3.089 (7)             | 121                     |
| C10—H10...O1 <sup>iv</sup>   | 0.93        | 2.45          | 3.314 (7)             | 154                     |
| C1—H1...O5 <sup>i</sup>      | 0.93        | 2.41          | 3.121 (7)             | 134                     |

Symmetry codes: (iii)  $x, y-1, z$ ; (ii)  $-x+2, -y+1, -z+2$ ; (iv)  $-x+3/2, y+1/2, -z+3/2$ ; (i)  $-x+2, -y, -z+2$ .

Fig. 1

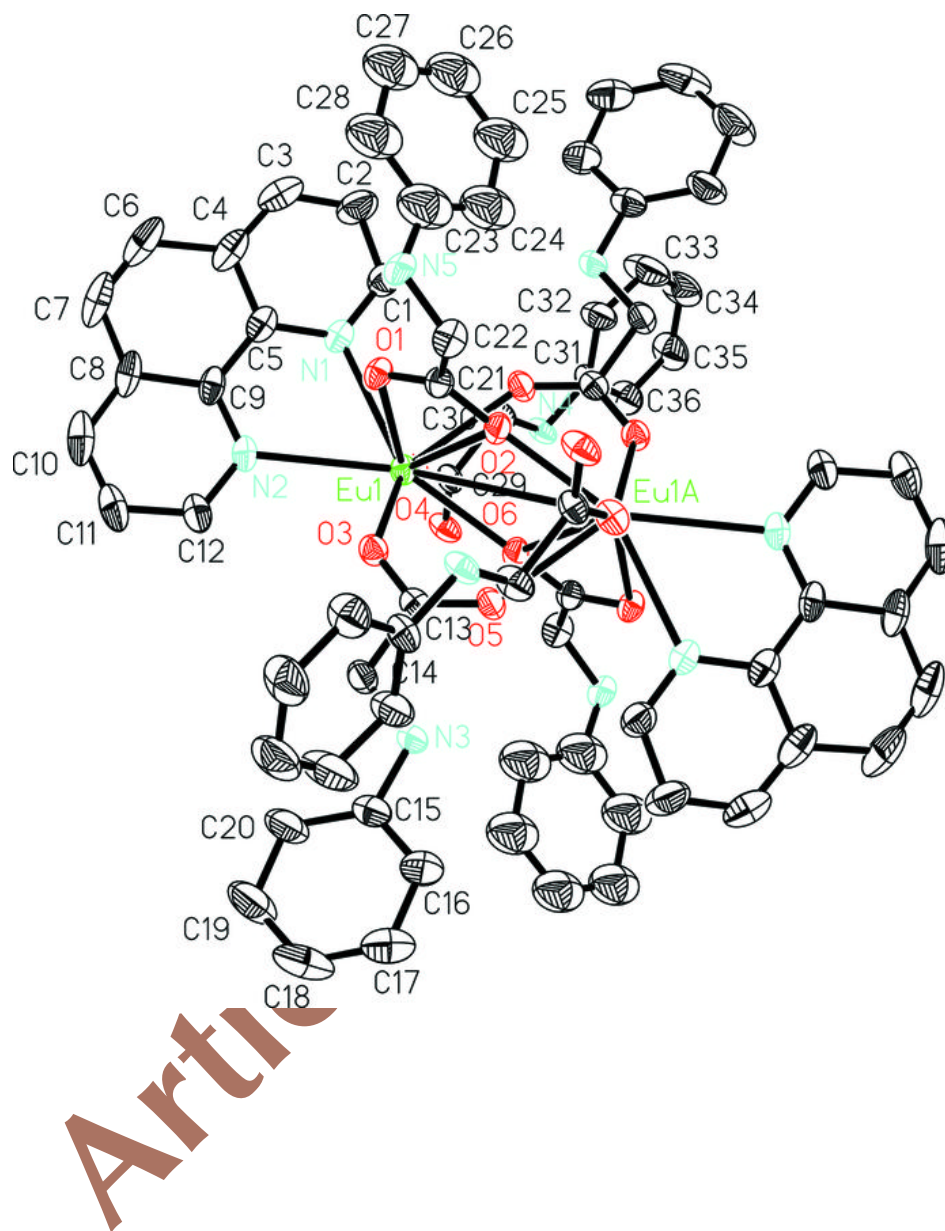
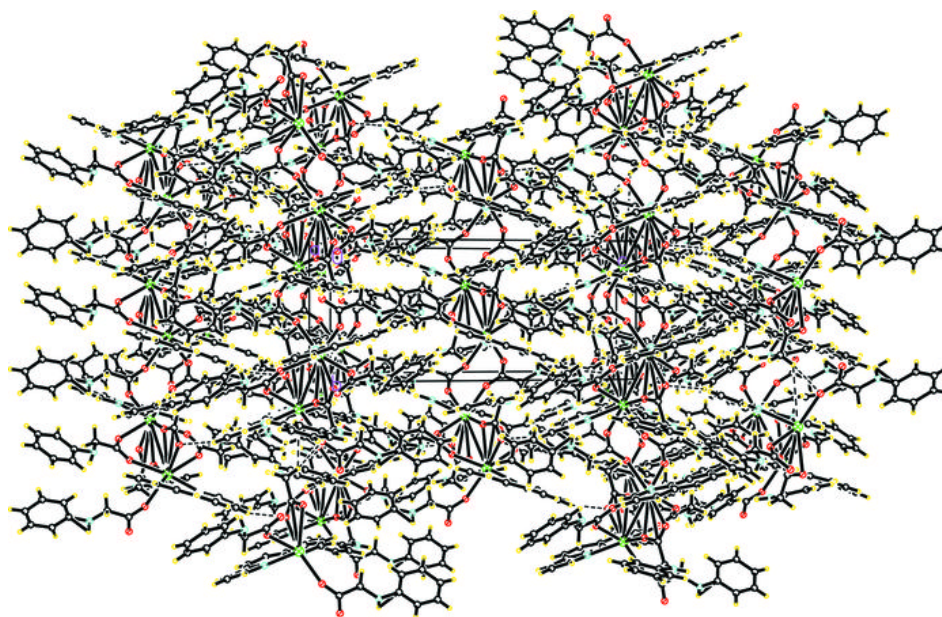


Fig. 2



Article retrá