Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# Poly[[hexaaquabis($\mu_3$-pyridine-2,5-dicarboxylato-$\kappa^4O$:$O'$,$N$:$O''$)bis($\mu_2$-pyridine-2,5-dicarboxylato-$\kappa^3O$:$O'$,$N$)dieuropium(III)copper(II)] dihydrate]

**Bao-Feng Zhang, Cheng-Zhi Xie, Xiao-Qing Wang,* Guang-Qiu Shen and De-Zhong Shen**

Department of Chemistry, Tsinghua University, Beijing 100084, People's Republic of China

Correspondence e-mail: xqwang@tsinghua.edu.cn

Received 14 October 2005
Accepted 9 January 2006

**Key indicators**

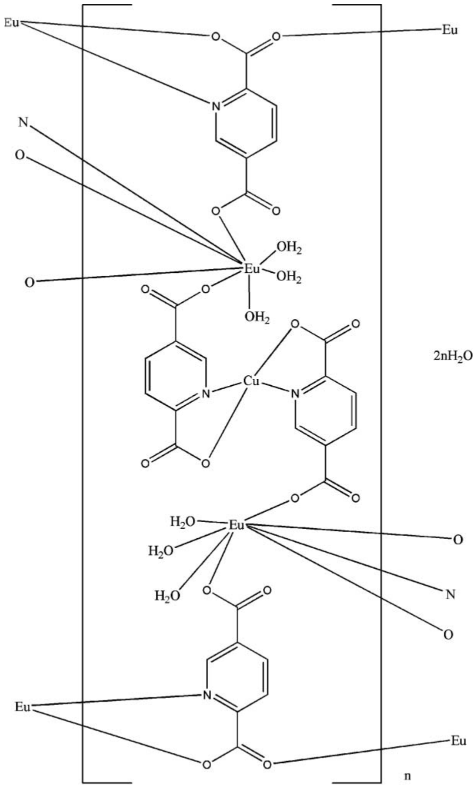
Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.005 Å
$R$ factor = 0.027
$wR$ factor = 0.061
Data-to-parameter ratio = 13.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title polymeric compound, $\{[Eu_2Cu(C_7H_3O_4)_4(H_2O)_6]\cdot 2H_2O\}_n$, was prepared by a hydrothermal reaction at 453 K. The $Eu^{III}$ ion has a double-capped trigonal prismatic coordination geometry with an $NdNO_7$ core, while the $Cu^{II}$ ion is located on an inversion center and assumes a square-planar coordination geometry. The pyridine-2,5-dicarboxylate dianions bridge the $Eu^{III}$ and $Cu^{II}$ ions, forming a three-dimensional polymeric structure.

## Comment

Lanthanide–transition metal complexes are currently of great interest because they are good models to investigate the nature of the magnetic exchange interactions between 3$d$ and 4$f$ metal ions (Lisowski & Starynowicz, 1999; Liang *et al.*, 2000, 2001). As part of our ongoing investigation on magnetic complexes containing lanthanide and transition metal ions, we present here the structure of the title polymeric $Eu^{III}$–$Cu^{II}$ complex, (I).



(I)

A segment of the three-dimensional polymeric structure of (I) is shown in Fig. 1. In the asymmetric unit there are one

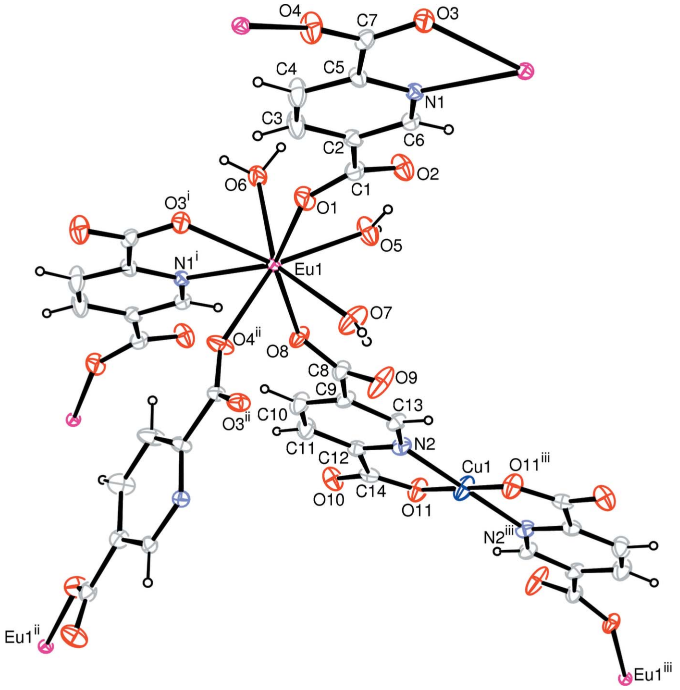


**Figure 1**

A segment of the polymeric structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). Uncoordinated water molecules have been omitted for clarity. [Symmetry codes: (i) $1 + x$, $y$, $z$; (ii) $1 + x$, $\frac{3}{2} - y$, $\frac{1}{2} + z$; (iii) $2 - x$, $2 - y$, $3 - z$.]

$Eu^{III}$ ion and one-half $Cu^{II}$ ion, located on an inversion center. The $Eu^{III}$ ion has a double-capped trigonal prismatic coordination geometry with an $NdNO_7$ core, involving three O atoms from three coordinated water molecules and four O atoms from four pyridine-2,5-dicarboxylate (pydc) dianions. The $Cu^{II}$ ion is chelated by two pydc ligands through their N and O atoms with a square-planar geometry. The Eu—O bonds range from 2.342 (3) to 2.435 (3) Å (Table 1). There are two independent pydc dianions in (I). While the C1-containig pydc dianion adopts a tetradentate chelating–bridging mode and links three $Eu^{III}$ ions, the C8-containing pydc dianion adopts a tridentate chelating–bridging coordination mode and links one $Eu^{III}$ and one $Cu^{II}$ ions. Thus, the pydc dianions link the Eu and Cu ions, forming a three-dimensional polymeric structure. The Eu$\cdots$Eu and Eu$\cdots$Cu separations between adjacent units are 6.406 (1) and 6.087 (3) Å, respectively.

Extensive O—H$\cdots$O hydrogen bonding occurs in the crystal structure of (I), and this stabilizes the crystal structure (Table 2).

## Experimental

A mixture of $Eu_2O_3$ (0.25 mmol), $Cu(ClO_4)_2\cdot 6H_2O$ (0.5 mmol), $H_2$pydc (1.0 mmol) and $H_2O$ (16.0 ml) was sealed in a 25 ml stainless steel reactor with a Teflon liner and heated directly to 453 K. After maintaining this temperature for 72 h, the reaction was cooled slowly to 303 K at a rate of 2 K h$^{-1}$. Blue crystals were obtained in 52% yield. Analysis calculated for $C_{28}H_{28}CuEu_2N_4O_{24}$ (%): C 28.67, H 2.39, N 4.78; found: C 28.73, H 2.31, N 4.81.

### *Crystal data*

$[Eu_2Cu(C_7H_3O_4)_4(H_2O)_6]\cdot 2H_2O$
$M_r = 1172.00$
Monoclinic, $P2_1/c$
$a = 9.271$ (3) Å
$b = 25.548$ (8) Å
$c = 7.793$ (2) Å
$\beta = 97.273$ (5)°
$V = 1831.0$ (9) Å$^3$
$Z = 2$
$D_x = 2.126$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 854 reflections
$\theta = 2.8$–26.2°
$\mu = 4.06$ mm$^{-1}$
$T = 293$ (2) K
Prism, blue
0.20 × 0.14 × 0.12 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{min} = 0.468$, $T_{max} = 0.610$
10493 measured reflections
3723 independent reflections
3242 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 26.4°$
$h = -11 \rightarrow 11$
$k = -30 \rightarrow 31$
$l = -4 \rightarrow 9$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.061$
$S = 1.06$
3723 reflections
268 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0272P)^2 + 2.202P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.47$ e Å$^{-3}$
$\Delta\rho_{min} = -1.19$ e Å$^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Eu1—O1 | 2.342 (3) | Eu1—O7 | 2.435 (3) |
| Eu1—O3$^{i}$ | 2.428 (3) | Eu1—O8 | 2.392 (3) |
| Eu1—O4$^{ii}$ | 2.347 (3) | Eu1—N1$^{i}$ | 2.589 (3) |
| Eu1—O5 | 2.409 (3) | Cu1—O11 | 1.946 (3) |
| Eu1—O6 | 2.397 (3) | Cu1—N2 | 1.967 (3) |
| | | | |
| O11—Cu1—N2$^{iii}$ | 96.42 (13) | | |

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

**Table 2**

Hydrogen-bond geometry (Å, °).

| $D$—H$\cdots$$A$ | $D$—H | H$\cdots$$A$ | $D\cdots A$ | $D$—H$\cdots$$A$ |
|---|---|---|---|---|
| O5—H5$A$$\cdots$O2 | 0.85 | 2.02 | 2.796 (4) | 152 |
| O5—H5$B$$\cdots$O10$^{iv}$ | 0.85 | 1.99 | 2.795 (4) | 159 |
| O6—H6$A$$\cdots$O10$^{v}$ | 0.86 | 1.90 | 2.756 (4) | 174 |
| O6—H6$B$$\cdots$O9$^{vi}$ | 0.84 | 1.84 | 2.671 (4) | 167 |
| O7—H7$A$$\cdots$O9 | 0.85 | 1.83 | 2.666 (4) | 169 |
| O7—H7$B$$\cdots$O12$^{vii}$ | 0.85 | 1.99 | 2.791 (5) | 158 |
| O12—H12$A$$\cdots$O1$^{viii}$ | 0.85 | 2.17 | 3.019 (5) | 174 |
| O12—H12$B$$\cdots$O3$^{i}$ | 0.85 | 2.06 | 2.888 (4) | 164 |

Symmetry codes: (i) $x + 1, y, z$; (iv) $-x + 2, -y + 2, -z + 2$; (v) $x - 1, y, z - 1$; (vi) $x, y, z - 1$; (vii) $x, y, z + 1$; (viii) $x, -y + \frac{3}{2}, z - \frac{1}{2}$.

H atoms were positioned geometrically and refined in the riding-model approximation, with C—H = 0.93 Å and O—H = 0.85 Å. $U_{iso}$(H) values were fixed at $1.2U_{eq}$(carrier). The deepest hole is located 1.42 Å from atom H6$B$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

**m298** Zhang *et al.* • $[Eu_2Cu(C_7H_3O_4)_4(H_2O)_6]\cdot 2H_2O$ *Acta Cryst.* (2006). E**62**, m297–m299

The work was financially supported by the National Natural Science Foundation of China (NO. 50132010) and the 985 Program of Tsinghua University, China.

## References

Bruker (1997). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (1999). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.

Bruker (2000). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Liang, Y. C., Cao, R., Su, W. P., Hong, M. C. & Zhang, W. J. (2000). *Angew. Chem. Int. Ed.* **39**, 3304–3307.

Liang, Y. C., Hong, M. C., Su, W. P., Cao, R. & Zhang, W. J. (2001). *Inorg. Chem.* **40**, 4574–4582.

Lisowski, J. & Starynowicz, P. (1999). *Inorg. Chem.* **38**, 1351–1355.

*Acta Cryst.* (2006). E**62**, m297–m299 Zhang *et al.* • $[Eu_2Cu(C_7H_3O_4)_4(H_2O)_6]\cdot 2H_2O$ **m299**