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catena-Poly[[aqua[3-(3-pyridyl)acrylato]europium(III)]-di-μ-3-(3-pyridyl)acrylato]

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.004 Å
R factor = 0.023
wR factor = 0.048
Data-to-parameter ratio = 16.1

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

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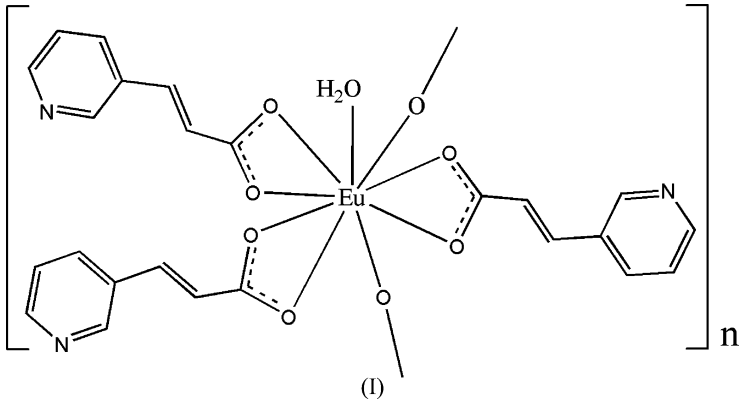
In the title compound, $[Eu(C_8H_6NO_2)_3(H_2O)]_n$, the europium(III) ion is coordinated by eight carboxylate O atoms and one water molecule. The carboxylate ligands bridge pairs of europium(III) ions, forming a zigzag chain along [100]; hydrogen bonds link the chains into sheets parallel to (001).

Comment

In recent years, research on metal–organic coordination polymers has been rapidly expanding because of their structural diversity and their potential applications as functional materials (Moulton *et al.*, 2001; Li *et al.*, 1998). The bifunctional ligand 3-pyridylacrylic acid (HTPA) is a potential multidentate ligand, and several types of complexes of HTPA have been studied (Zhang *et al.*, 2000; Ayyappan *et al.*, 2001; Gunning *et al.*, 2005). Until now, however, only a few crystallographic studies of 4*f*-block metal complexes of HTPA have been reported (Gunning *et al.*, 2005).



(I)

Here, we report the synthesis and structure of the title complex, $[Eu(TPA)_3(H_2O)]_n$ (I) (Fig. 1), whose structure consists of a repeating unit of formula $[Eu(C_8H_6NO_2)_3(H_2O)]$. Each Eu^{III} centre is coordinated by eight carboxylate O atoms and one water molecule. The europium(III) ions are joined into a coordination polymer chain along [100], reinforced by O—H···O hydrogen bonds (Table 1). Adjacent [100] chains are linked by O—H···N hydrogen bonds, forming sheets parallel to (001) (Fig. 2).

Experimental

A mixture of $EuCl_3{\cdot}6H_2O$ (0.2 mmol), 3-pyridylacrylic acid (0.2 mmol), H_2O (5 ml), and 0.65 *M* NaOH aqueous solution (0.2 ml, 0.13 mmol) was sealed in a 25 ml Teflon-lined stainless reactor and heated at 393 K for 72 h under autogenous pressure, then cooled at a rate of 10 K every 3 h to 373 K, followed by slow cooling to room

temperature, when a few colourless crystals were obtained. Analysis: found C 47.2, H 3.3, N 7.2%; $C_{24}H_{20}EuN_3O_7$ requires C 46.9, H 3.3, N 6.8%.

Crystal data

$[Eu(C_8H_6NO_2)_3(H_2O)]$
M_r = 614.39
Triclinic, $P\overline{1}$
a = 6.2459 (6) Å
b = 12.7698 (13) Å
c = 15.7220 (16) Å
α = 111.7710 (10)°
β = 90.3200 (10)°
γ = 95.1760 (10)°
V = 1158.7 (2) Å^3
Z = 2
D_x = 1.761 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.76 mm^{-1}
T = 291 (2) K
Block, colourless
0.15 × 0.09 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.675, T_{max} = 0.799
10024 measured reflections
5207 independent reflections
4755 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.048
S = 1.04
5207 reflections
324 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0184P)^2 + 0.2729P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H1W···O3^{i}	0.821 (17)	1.946 (17)	2.765 (3)	175 (3)
O7—H2W···N1^{ii}	0.840 (17)	1.901 (18)	2.731 (3)	170 (4)

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

All H atoms were positioned geometrically and treated as riding atoms with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

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: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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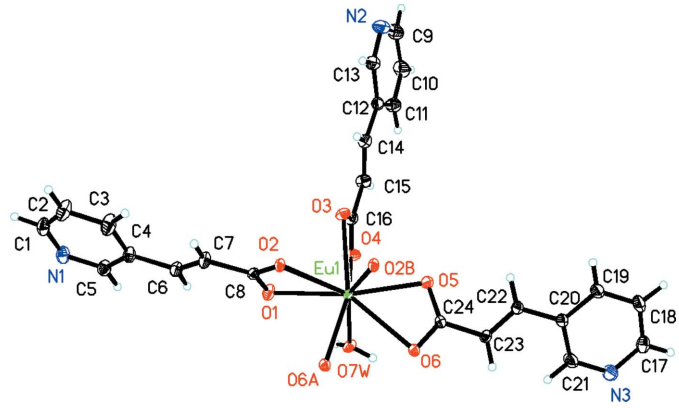

Figure 1
The coordination environment of the Eu^{III} ion in (I), with displacement ellipsoids drawn at the 30% probability level. [Symmetry codes: (A) $-x$, $1-y$, $1-z$; (B) $1-x$, $1-y$, $1-z$.]

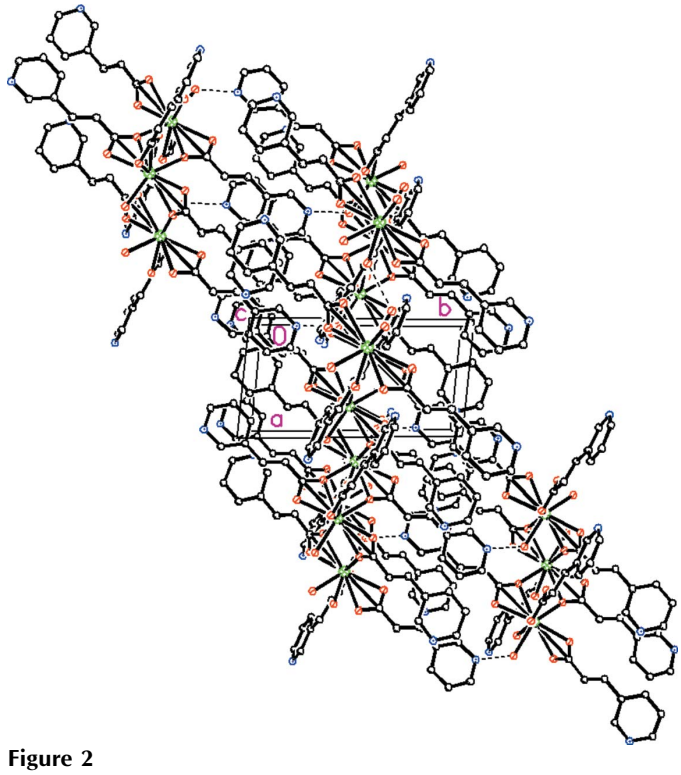

Figure 2
A packing diagram, viewed along the c axis. All H atoms have been omitted for clarity. Dashed lines indicate hydrogen bonds.

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