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## Key indicators

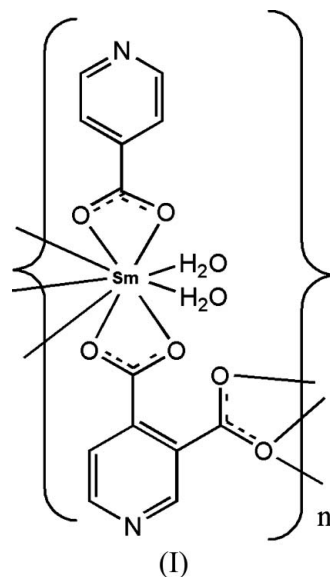
Single-crystal X-ray study  
 $T = 293$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
Disorder in main residue  
 $R$  factor = 0.025  
 $wR$  factor = 0.062  
Data-to-parameter ratio = 12.2For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.**catena-Poly[bis[di aquaisonicotinosamarium(III)]-  
bis( $\mu_3$ -pyridine-3,4-dicarboxylato)]**

The title samarium(III) coordination polymer,  $[\text{Sm}(\text{C}_6\text{H}_4\text{NO}_2)(\text{C}_7\text{H}_3\text{NO}_4)(\text{H}_2\text{O})_2]_n$ , has a pyridine-3,4-dicarboxylate-bridged ribbon structure. The isonicotinate (ina) anion chelates to the water-coordinated metal atom, which shows ninefold coordination. The ina unit arises from the decarboxylation of pyridine-3,4-dicarboxylic acid under the hydrothermal conditions of the synthesis.

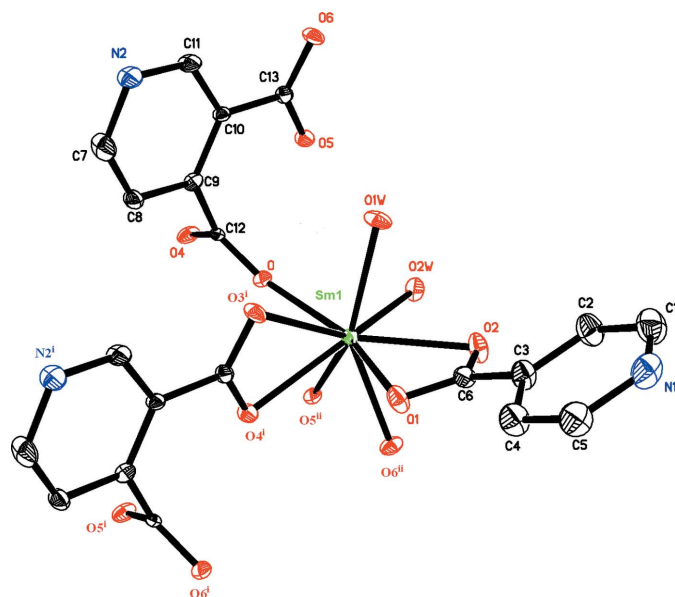
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## Comment

In our previous work, three lanthanide coordination polymers, *viz.*  $[\text{Nd}(\text{pydc})_2 \cdot \text{H}_2\text{O}]_n$ ,  $[\text{Eu}(\text{pydc})(\text{ina})(\text{H}_2\text{O})_2]_n$  and  $[\text{Gd}(\text{pydc})(\text{ina})(\text{H}_2\text{O})_2]_n$  (pydc = pyridine-3,4-dicarboxylate and ina = isonicotinate), were synthesized by treating  $\text{Ln}^{\text{III}}$  nitrate with pyridine-3,4-dicarboxylic acid under similar reaction conditions (Han *et al.*, 2005, 2006). Unexpectedly, decarboxylation occurred and the pydc group was transformed into an ina group in the hydrothermal syntheses of the  $\text{Eu}^{\text{III}}$  and  $\text{Gd}^{\text{III}}$  coordination polymers. This study has been extended to other  $\text{Ln}^{\text{III}}$  coordination polymers as the basis for investigating *in situ* decarboxylation. We report here the synthesis and structure of the samarium(III) analog, (I).



In (I), the  $\text{Sm}^{\text{III}}$  ion is coordinated by nine O atoms, five from three pydc ligands, two from one chelating ina group and two from two aqua ligands (Fig. 1). Pairs of Sm atoms are bridged by two  $\mu_2$ -carboxylate O atoms of the pydc groups, forming dinuclear  $\text{Sm}_2(\text{pydc})_2$  subunits which are interconnected through the chelating carboxylate groups of the pydc ligands, forming an infinite one-dimensional ribbon; the


**Figure 1**

Plot depicting the coordination environment of the metal atom, the asymmetric unit, together with additional ligands to complete the metal coordination, with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $-x + 2, -y + 1, -z + 1$ .]

Sm $\cdots$ Sm distances are 5.954 (3) and 6.437 (3) Å. These chains are further linked *via* hydrogen bonds (Table 2) between pyridyl N atoms, carboxylate O atoms and aqua ligands, forming a three-dimensional supramolecular network.

As for [Eu(pydc)(ina)(H<sub>2</sub>O)<sub>2</sub>]<sub>n</sub> and [Gd(pydc)(ina)(H<sub>2</sub>O)<sub>2</sub>]<sub>n</sub>, decarboxylation also occurred in the samarium(III) coordination polymer and the pydc groups were partially transformed into ina groups.

## Experimental

A mixture of Sm(NO<sub>3</sub>)<sub>3</sub>·6H<sub>2</sub>O (0.5 mmol, 0.222 g), pyridine-3,4-dicarboxylic acid (0.5 mmol, 0.087 g), NaOH (1 mmol, 0.04 g) and water (10 ml) was placed in a 23 ml Teflon reactor, which was heated at 453 K for 6 d. The reactor was cooled to room temperature at a rate of 5 K h<sup>-1</sup> (yield 60%). Analysis for C<sub>13</sub>H<sub>11</sub>N<sub>2</sub>O<sub>8</sub>Sm (found/calc): C 32.85/32.97, H 2.39/2.34, N 5.78/5.92%.

### Crystal data

[Sm(C <sub>6</sub> H <sub>4</sub> NO <sub>2</sub> )(C <sub>7</sub> H <sub>3</sub> NO <sub>4</sub> )(H <sub>2</sub> O) <sub>2</sub> ]	$Z = 4$
$M_r = 473.59$	$D_x = 1.915 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 5.9541 (19) \text{ \AA}$	$\mu = 3.62 \text{ mm}^{-1}$
$b = 25.047 (8) \text{ \AA}$	$T = 293 (2) \text{ K}$
$c = 11.215 (4) \text{ \AA}$	Block, colorless
$\beta = 100.775 (7)^\circ$	$0.37 \times 0.35 \times 0.23 \text{ mm}$
$V = 1643.0 (9) \text{ \AA}^3$	

### Data collection

Bruker APEX area-detector diffractometer	9867 measured reflections
$\varphi$ and $\omega$ scans	3228 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3049 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.348, T_{\max} = 0.490$ (expected range = 0.309–0.435)	$R_{\text{int}} = 0.027$
	$\theta_{\text{max}} = 26.0^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.025$   
 $wR(F^2) = 0.062$   
 $S = 1.07$   
 3228 reflections  
 264 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0254P)^2 + 3.8278P]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.58 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.81 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Sm1—O1W	2.363 (3)	Sm1—O4 <sup>ii</sup>	2.470 (3)
Sm1—O2W	2.370 (3)	Sm1—O2	2.492 (3)
Sm1—O3	2.394 (2)	Sm1—O6 <sup>i</sup>	2.509 (3)
Sm1—O5 <sup>i</sup>	2.420 (2)	Sm1—O3 <sup>ii</sup>	2.643 (3)
Sm1—O1	2.463 (3)		
O1W—Sm1—O2W	76.56 (11)	O3—Sm1—O1	152.40 (9)
O1W—Sm1—O3	83.82 (10)	O5 <sup>i</sup> —Sm1—O1	79.68 (9)
O2W—Sm1—O3	80.03 (9)	O3—Sm1—O4 <sup>ii</sup>	115.23 (8)
O1W—Sm1—O5 <sup>i</sup>	127.79 (9)	O5 <sup>i</sup> —Sm1—O4 <sup>ii</sup>	81.96 (9)
O3—Sm1—O5 <sup>i</sup>	80.60 (9)	O1—Sm1—O4 <sup>ii</sup>	80.78 (10)

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

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1WB $\cdots$ N2 <sup>iii</sup>	0.843 (18)	1.84 (2)	2.683 (4)	172 (5)
O1W—H1WA $\cdots$ O1 <sup>iv</sup>	0.837 (19)	1.95 (2)	2.761 (4)	164 (4)
O2W—H2WA $\cdots$ N1 <sup>v</sup>	0.844 (19)	1.86 (3)	2.69 (2)	167 (7)
O2W—H2WA $\cdots$ N1 <sup>v</sup>	0.844 (19)	1.93 (3)	2.76 (2)	167 (6)
O2W—H2WB $\cdots$ O4 <sup>vi</sup>	0.837 (19)	2.28 (4)	2.908 (4)	132 (4)
O2W—H2WB $\cdots$ O5 <sup>vi</sup>	0.837 (19)	2.29 (3)	2.997 (4)	143 (5)

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

Carbon-bound H atoms were placed at calculated positions and refined in the riding-model approximation ( $C-H = 0.93 \text{ \AA}$ ), with  $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ . Water H atoms were located in difference Fourier maps and refined, with distance restraints of  $O-H = 0.85 (2) \text{ \AA}$  and  $H\cdots H = 1.39 (1) \text{ \AA}$ . The pyridine ring of the isonicotinate group is disordered; the occupancy was fixed at 0.5. Distance restraints  $C-C = C-N = 1.390 (5) \text{ \AA}$  and  $C\cdots C = C\cdots N = 2.780 (5) \text{ \AA}$  were applied.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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, 2001); software used to prepare material for publication: *SHELXTL*.

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