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Poly[tris[μ_2-3-(3-pyridyl)acrylato]samarium(III)]

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Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.009 Å
R factor = 0.052
wR factor = 0.116
Data-to-parameter ratio = 14.3

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

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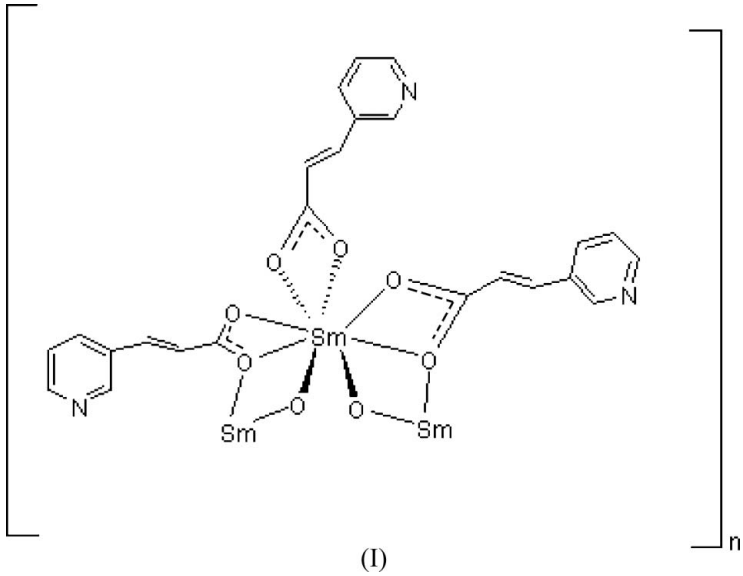
In the title compound, $[Sm(C_8H_6NO_2)_3]_n$, the Sm^{III} atom has an irregular polyhedral geometry. It is eight-coordinated by one bidentate and two tridentate 3-(3-pyridyl)acrylate acid (3-HPYA) ligands bridging the two symmetry-related Sm^{III} centres, which results in the formation of a one-dimensional zigzag chain.

Comment

Currently there is considerable interest in metal-organic coordination polymers with fascinating network topologies and specific properties for potential applications in the fields of molecular magnetism, electrical conductivity and photoluminescence, as well as in inclusion chemistry, molecular recognition and catalysis (Evans *et al.*, 1999; Moulton & Zaworotko, 2001; Li *et al.*, 2004; Tabares *et al.*, 2001). The coordination chemistry of aromatic carboxylates with rare earth metal complexes has received considerable attention due to the variety of bridging abilities of carboxylates (Thirumurugan & Natarajan, 2004). Many such crystalline coordination polymers with one-, two- and three-dimensional structures have been produced by successful synthesis of coordination polymers (Zhou *et al.*, 2004; Gunning & Cahill, 2005) using rare earth metals and the 3-(3-pyridyl)acrylate acid (3-HPYA) ligand. We synthesized another rare earth metal coordination polymer using the 3-HPYA ligand and samarium(III) nitrate and report here its crystal structure.



(I)

As illustrated in Fig. 1, the Sm^{III} atom is eight-coordinated by one bidentate and two tridentate 3-HPYA ligands bridging

the two symmetry-related Sm^{III} centres, which results in the formation of a one-dimensional zigzag chain (Fig. 2). The central Sm^{III} atom is linked to the ligands by Sm—O bonds ranging from 2.421 (4) to 2.567 (4) Å [average Sm—O distance = 2.479 (4) Å; Table 1], and has an irregular polyhedral geometry.

Dipole–dipole and van der Waals interactions are effective in the molecular packing.

Experimental

For the preparation of the title compound, a mixture of $Sm(NO_3)_3{\cdot}6H_2O$ (0.110 g, 0.25 mmol), 3-(3-pyridyl)acrylic acid (0.075 g, 0.50 mmol), sodium hydroxide (0.020 g, 0.50 mmol) and water (10 ml) were sealed in a 23 ml Teflon-lined stainless steel Parr bomb. The bomb was heated to 403 K for 2 d and then it was cooled to room temperature at 10 K h^{-1} to give colourless crystals of (I) (yield 0.069 g, 70%).

Crystal data

$[Sm(C_8H_6NO_2)_3]$
M_r = 594.76
Triclinic, $P\overline{1}$
a = 6.2302 (13) Å
b = 12.712 (3) Å
c = 15.650 (3) Å
α = 111.814 (4)°
β = 90.354 (4)°
γ = 95.088 (4)°
V = 1145.1 (4) Å^3
Z = 2
D_x = 1.725 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.61 mm^{-1}
T = 294 (2) K
Block, colourless
0.32 × 0.25 × 0.18 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.45, T_{max} = 0.62
6220 measured reflections
4387 independent reflections
3742 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 26.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.116
S = 1.04
4387 reflections
307 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 1.2P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.97 e Å^{-3}
$\Delta\rho_{min}$ = −1.56 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sm1—O3	2.421 (4)	Sm1—O1	2.478 (4)
Sm1—O6^{i}	2.429 (4)	Sm1—O4	2.510 (4)
Sm1—O2^{ii}	2.431 (4)	Sm1—O2	2.544 (4)
Sm1—O5	2.453 (4)	Sm1—O6	2.567 (4)

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

H atoms were positioned geometrically, with C—H = 0.93 Å and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C). The deepest residual density hole is 0.59 Å from atom Sm1.

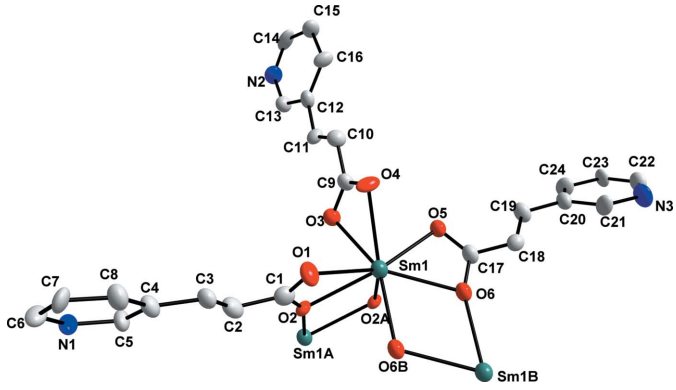


Figure 1
The asymmetric unit of (I), together with additional atoms to complete the coordination of Sm1 and the carboxylate bridge, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry codes: (A) $1-x, -y, -z$; (B) $2-x, -y, -z$].

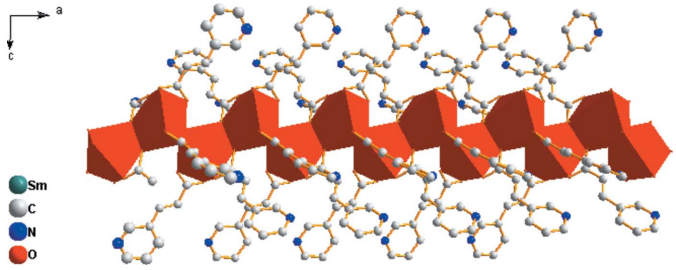


Figure 2
A view of the one-dimensional zigzag chain. H atoms have been omitted for clarity.

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

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