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catena-Poly[[[diaqua(6-carboxypyridine-2-carboxylato-κ^3N,O,O')samarium(III)]-μ-pyridine-2,6-dicarboxylato-$\kappa^4N,O,O':O''$] tetrahydrate]

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In the title complex, $[Sm(C_7H_3O_4)(C_7H_4O_4)(H_2O)_2]\cdot4H_2O$, the coordination number of the Sm atom is nine. The pyridine-2,6-dicarboxylate ligand chelates to the Sm atom and bridges to the neighbouring Sm atoms to form infinite chains along the *c* axis.

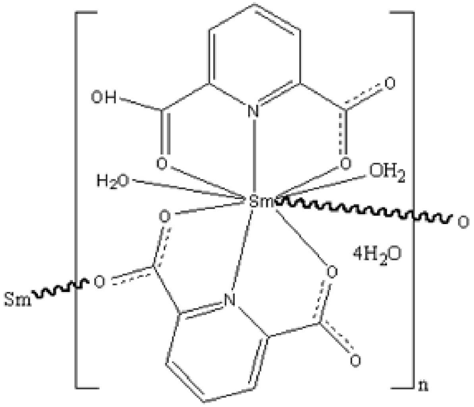
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.012 Å
R factor = 0.062
wR factor = 0.156
Data-to-parameter ratio = 13.7

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

Comment

In recent years, the use of lanthanide elements for constructing metal–organic framework (MOF) structures has attracted a lot of interest due to their high coordination numbers, along with special magnetic and luminescent properties (Benelli & Gatteschi, 2002; Ghosh & Bharadwaj, 2003). A search of the Cambridge Structural Database (February 2005 update; Allen, 2002) for pyridine-2,6-dicarboxylic acid ($pydcH_2$) or the deprotonated ligand ($pydcH^{-1}$ or $pydc^{2-}$) coordinated to samarium yielded only five hits. The title compound, (I), which is a novel linear coordination polymer of samarium with pyridine-2,6-dicarboxylate ligands, is reported here.



(I)

The asymmetric unit of (I) is composed of one Sm^{III} ion, one $PydcH^{-1}$ and one $Pydc^{2-}$ ligand, two coordinated water molecules and four water molecules of crystallization. Atom Sm1 is coordinated by $pydcH^-$ (atoms O1, N1 and O3), $pydc^{2-}$ (O6, N2 and O7), and two aqua ligands (O9 and O10); the Sm atom is also bonded to one bridging atom, $O5^{iii}$ [symmetry code: (iii) x, y, $z - 1$], from a neighbouring $pydc^{2-}$ ligand, giving an overall nine-coordination (Fig. 1). The $pydc^{2-}$ group chelates to the Sm1 atom and bridges to the neighbouring $Sm1^i$ atom [symmetry code: (i) x, $\frac{3}{2} - y$, $z + \frac{1}{2}$], forming an infinite chain along the *c* axis (Fig. 2). Two neighbouring chains are linked to form a ladder-like band through O—H$\cdots$O hydrogen bonds (Table 2 and Fig. 3). The ladder-like

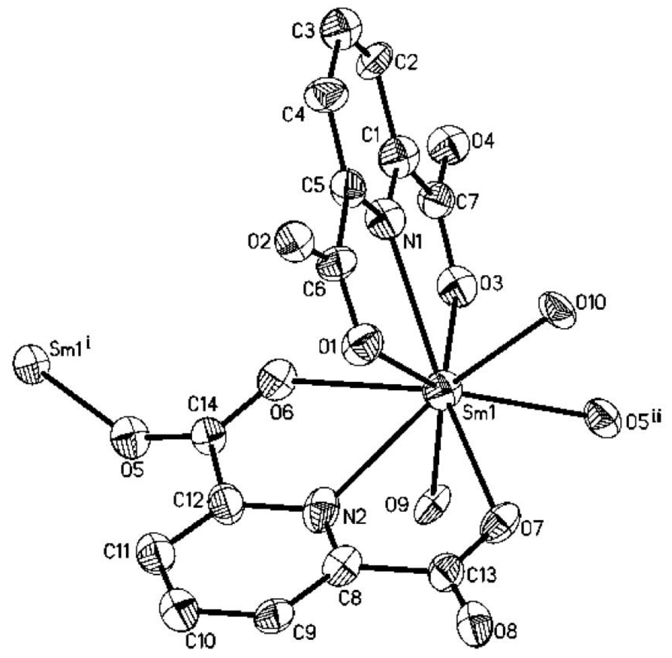


Figure 1
The structure of (I), with displacement ellipsoids drawn at the 50% probability level. All H atoms and uncoordinated water molecules have been omitted for clarity. [Symmetry codes: (i) $x, \frac{3}{2} - y, z + \frac{1}{2}$; (ii) $x, \frac{3}{2} - y, z - \frac{1}{2}$.]

bands form a layer structure parallel to (100) by hydrogen bonds with the uncoordinated water molecules, and adjacent layers are linked together through hydrogen bonds, resulting in a three-dimensional framework.

Experimental

Sm_2O_3 was acquired from Aldrich, and pyridine-2,6-dicarboxylic acid was synthesized according to the literature (Singer & McElvain, 1935). To a solution of pyridine-2,6-dicarboxylic acid (167 mg, 1 mmol) in water (60 ml) and sodium hydroxide (1 *M*, 2 ml), Sm_2O_3 (349 mg, 1 mmol) was added. The mixture was stirred at 373 K for 12 h and then filtered. Single crystals of (I) suitable for X-ray analysis were grown from the filtrate after six weeks (yield 65%). Compound (I) is stable in air and soluble in water.

Crystal data

$C_{14}H_{11}N_2O_{10}Sm \cdot 4H_2O$
$M_r = 589.66$
Monoclinic, $P2_1/c$
$a = 13.973$ (3) Å
$b = 11.203$ (2) Å
$c = 12.830$ (3) Å
$\beta = 102.367$ (4)°
$V = 1961.8$ (7) Å^3
$Z = 4$

$D_x = 1.996$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 935 reflections
$\theta = 2.4$–25.6°
$\mu = 3.07$ mm^{-1}
$T = 293$ (2) K
Prism, colourless
0.20 × 0.14 × 0.12 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\min} = 0.61$, $T_{\max} = 0.69$
10 285 measured reflections

3846 independent reflections
2849 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.044$
$\theta_{\max} = 26.0°$
$h = -16 \rightarrow 17$
$k = -13 \rightarrow 13$
$l = -13 \rightarrow 15$

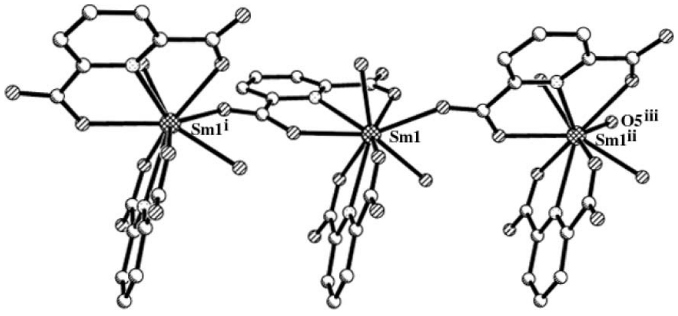


Figure 2
The infinite chain along the *c* axis. [Symmetry codes: (i) x, $\frac{3}{2} - y, z + \frac{1}{2}$; (ii) $x, \frac{3}{2} - y, z - \frac{1}{2}$; (iii) $x, y, z - 1$.]

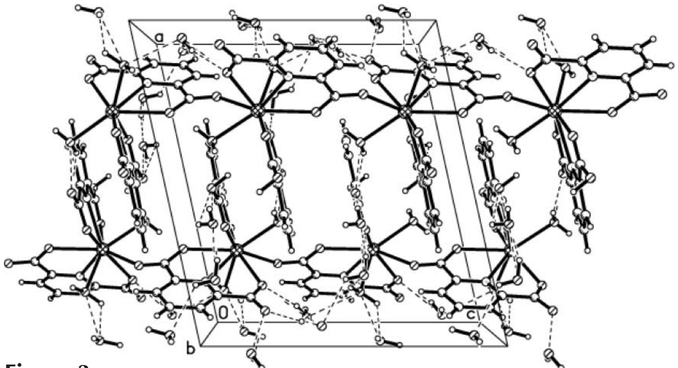


Figure 3
The crystal packing of (I), viewed down the *b* axis. Dashed lines indicate hydrogen bonds.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.156$
$S = 1.06$
3846 reflections
280 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.09P)^2 + 1.99P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.98$ e Å^{-3}
$\Delta\rho_{\min} = -2.01$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sm1—O9	2.388 (5)	Sm1—O6	2.524 (6)
Sm1—O10	2.423 (6)	Sm1—N2	2.537 (8)
Sm1—O3	2.426 (6)	Sm1—O1	2.537 (6)
Sm1—O5^i	2.446 (6)	Sm1—N1	2.556 (7)
Sm1—O7	2.476 (6)		
O9—Sm1—O10	141.5 (2)	O5^i—Sm1—N2	128.9 (2)
O9—Sm1—O3	79.90 (19)	O7—Sm1—N2	62.3 (2)
O10—Sm1—O3	97.26 (19)	O6—Sm1—N2	62.5 (2)
O9—Sm1—O5^i	71.6 (2)	O9—Sm1—O1	141.0 (2)
O10—Sm1—O5^i	70.7 (2)	O10—Sm1—O1	71.2 (2)
O3—Sm1—O5^i	74.65 (19)	O3—Sm1—O1	124.7 (2)
O9—Sm1—O7	86.04 (18)	O5^i—Sm1—O1	139.1 (2)
O10—Sm1—O7	78.56 (19)	O7—Sm1—O1	81.21 (18)
O3—Sm1—O7	151.38 (19)	O6—Sm1—O1	84.23 (19)
O5^i—Sm1—O7	77.3 (2)	N2—Sm1—O1	65.8 (2)
O9—Sm1—O6	72.88 (19)	O9—Sm1—N1	133.5 (2)
O10—Sm1—O6	143.9 (2)	O10—Sm1—N1	73.3 (2)
O3—Sm1—O6	75.08 (19)	O3—Sm1—N1	62.4 (2)
O5^i—Sm1—O6	136.45 (19)	O5^i—Sm1—N1	118.5 (2)
O7—Sm1—O6	124.2 (2)	O7—Sm1—N1	139.4 (2)
O9—Sm1—N2	75.5 (2)	O6—Sm1—N1	72.0 (2)
O10—Sm1—N2	124.8 (2)	N2—Sm1—N1	112.5 (2)
O3—Sm1—N2	135.5 (2)	O1—Sm1—N1	62.4 (2)

Symmetry code: (i) $x, \frac{3}{2} - y, z - \frac{1}{2}$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*A*···O3^{ii}	0.96	2.60	3.515 (9)	161
O9—H9*A*···O12	0.96	2.50	3.295 (8)	140
O9—H9*C*···O14^{iii}	0.96	2.03	2.720 (7)	127
O10—H10*A*···O6^{i}	0.85	2.13	2.707 (8)	125
O10—H10*C*···O1	0.85	2.48	2.889 (8)	111
O10—H10*C*···O4^{ii}	0.85	2.01	2.720 (9)	141
O11—H11*B*···O7	0.85	2.08	2.912 (8)	164
O12—H12*A*···O14^{iv}	0.85	2.39	3.004 (9)	130
O12—H12*B*···O3	0.85	2.52	2.945 (8)	112
O12—H12*B*···O13	0.85	2.07	2.775 (8)	140
O13—H13*B*···O4	0.85	1.87	2.642 (8)	150
O14—H14*B*···O8^{v}	0.95	1.73	2.683 (8)	176
O14—H14*C*···O11^{v}	0.86	2.17	2.895 (8)	142

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

O-bound H atoms were located from difference density maps (O—H = 0.85–0.96 Å) and C-bound H atoms were positioned geometrically (C—H = 0.93 Å). All H atoms were refined as riding, with isotropic displacement parameters 1.2 times the $U_{\rm eq}$ value of the parent atom. The maximum and minimum electron-density peaks are located 1.17 and 0.55 Å, respectively, from atom Sm1.

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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