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Crystal structure of poly[aqua-(μ_3 -4-(pyridin-4-yl)isophthalato- κ^4 O,O':O'':O''')-(μ_2 -5-carboxy-2-(pyridin-4-yl)benzoato- κ^2 O:O')samarium(III)], $C_{26}H_{18}N_2O_9Sm$

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.41 × 0.35 × 0.28 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	2.54 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω -scans
$\theta_{\max}$, completeness:	25.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	46473, 4404, 0.063
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3906
$N(\text{param})_{\text{refined}}$:	345
Programs:	CrysAlis ^{PRO} [1], SHELX [2, 3]

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sm1	0.21398(2)	0.49110(2)	0.262715(7)	0.01830(7)
N1	0.1595(4)	0.2396(4)	0.43874(13)	0.0326(9)
N2	0.8882(4)	0.9146(4)	0.33975(14)	0.0383(9)
O1	0.4458(3)	0.5375(3)	0.22759(11)	0.0376(8)
H1A	0.4583	0.6284	0.2244	0.056*
H1B	0.4430	0.4978	0.2001	0.056*
O2	0.3371(3)	0.6563(3)	0.31188(10)	0.0359(8)
O3	0.3320(4)	0.8932(3)	0.31319(10)	0.0396(8)
O4	−0.0083(4)	0.6754(4)	0.46205(12)	0.0601(11)
O5	0.0959(3)	0.8011(4)	0.52257(11)	0.0440(9)
H5	0.0140	0.7894	0.5327	0.066*
O6	1.0103(3)	0.3319(3)	0.27961(10)	0.0280(7)
O7	1.0732(3)	0.4985(3)	0.33243(10)	0.0380(8)
O8	0.3371(3)	0.2765(3)	0.28781(10)	0.0347(7)
O9	0.5044(3)	0.1207(3)	0.26890(12)	0.0429(8)
C1	0.0961(5)	0.7410(5)	0.48089(16)	0.0313(10)
C2	0.2388(4)	0.7634(4)	0.45797(14)	0.0233(9)
C3	0.3722(5)	0.8004(5)	0.48388(14)	0.0290(10)
H3	0.3752	0.8110	0.5165	0.035*
C4	0.5011(5)	0.8215(5)	0.46083(14)	0.0295(10)
H4	0.5909	0.8419	0.4786	0.035*
C5	0.4985(4)	0.8125(4)	0.41164(13)	0.0205(8)
C6	0.3632(4)	0.7750(4)	0.38585(13)	0.0203(8)
C7	0.2354(4)	0.7480(4)	0.40945(14)	0.0228(9)
H7	0.1472	0.7195	0.3923	0.027*
C8	0.6356(4)	0.8444(4)	0.38710(14)	0.0223(9)
C9	0.7227(5)	0.9639(5)	0.39966(16)	0.0335(10)
H9	0.6992	1.0223	0.4244	0.040*
C10	0.8442(5)	0.9947(5)	0.37499(18)	0.0405(12)

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Abstract

$C_{26}H_{18}N_2O_9Sm$, monoclinic $P2_1/n$ (no. 14), $a = 8.9665(3)$ Å, $b = 9.3617(3)$ Å, $c = 28.3925(9)$ Å, $\beta = 95.134(3)^\circ$, $V = 2373.76(12)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0317$, $wR_{\text{ref}}(F^2) = 0.0637$, $T = 293(2)$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

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Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
H10	0.8993	1.0764	0.3834	0.049*
C11	0.8072(5)	0.7978(5)	0.32895(15)	0.0344(11)
H11	0.8371	0.7386	0.3052	0.041*
C12	0.6811(5)	0.7593(4)	0.35099(14)	0.0278(10)
H12	0.6276	0.6775	0.3417	0.033*
C13	0.3437(4)	0.7742(4)	0.33284(14)	0.0241(9)
C14	0.4681(4)	0.2242(4)	0.29244(14)	0.0242(9)
C15	0.5852(4)	0.2896(4)	0.32741(13)	0.0182(8)
C16	0.5619(4)	0.3359(4)	0.37327(14)	0.0217(9)
C17	0.6786(4)	0.4061(4)	0.39990(14)	0.0263(9)
H17	0.6643	0.4370	0.4303	0.032*
C18	0.8154(4)	0.4305(4)	0.38190(14)	0.0260(9)
H18	0.8907	0.4799	0.3997	0.031*
C19	0.8389(4)	0.3805(4)	0.33712(14)	0.0225(9)
C20	0.7248(4)	0.3096(4)	0.31065(14)	0.0229(9)
H20	0.7418	0.2745	0.2810	0.027*
C21	0.4218(4)	0.3040(4)	0.39592(13)	0.0201(8)
C22	0.3524(4)	0.1707(4)	0.39032(14)	0.0255(9)
H22	0.3930	0.1005	0.3721	0.031*
C23	0.2235(5)	0.1437(5)	0.41191(16)	0.0318(10)
H23	0.1788	0.0545	0.4076	0.038*
C24	0.2278(5)	0.3669(5)	0.44465(16)	0.0347(11)
H24	0.1858	0.4347	0.4634	0.042*
C25	0.3564(5)	0.4023(4)	0.42438(15)	0.0288(10)
H25	0.3996	0.4918	0.4297	0.035*
C26	0.9833(4)	0.4047(4)	0.31549(14)	0.0230(9)

Source of material

A mixture of Sm(NO₃)₃·6H₂O (0.1331 g, 0.3 mmol), 4-(pyridin-4-yl)-isophthalic acid (0.1 mmol, 24.3 mg), a few drops of a diluted NaOH solution and distilled water (10 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner at 443 K for 28 h, followed by slow cooling to room temperature. Colourless crystals of the title compound formed.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms. *U*_{iso} parameters of the H atoms were fixed depending of the *U*_{eq} parameter of the corresponding parent non-hydrogen atom.

Discussion

Research on coordination complexes has made considerable progress in the fields of supramolecular chemistry and crystal engineering and functional applications. The observation of coordination complexes constructed from organic ligands and metal ions through a self-assembly route has been explored intensively, and many efforts have been devoted to use of N- and O-donor organic ligands as co-ligands to bridge

metalions to form one-dimensional (1D) chain structures and 2- or 3-D networks [4, 5]. However, it is still a great challenge in crystal engineering to obtain designed and predictable frameworks with potential properties assembled by coordination bonds and/or weak supramolecular interactions such as hydrogen bonds, π–π stacking, and host-guest ionic interactions. This contribution is part of our general interest in this field [6–10].

The asymmetric unit of the title structure contains one Sm(III) metal, one water molecules and organic mono-anion as a bridging ligand and a dianionic ligand as a threefold bridging ligand (*cf.* the name and the figure) to construct a coordination polymer. The samarium atom is seven-coordinated by one water ligand, six oxygen atoms from five organic ligands. A two-dimensional coordination polymer is obtained, a fact that is typical for coordination polymers constructed from oligocarboxylate ligands [11, 12]. The Sm–O2 bond length is 2.298(3) Å, the Sm–O6 bond length is 2.438(3) Å, the Sm–O8 bond length is 2.371(3). The bond angles of O–Sm–O are in the range of 53.61(9)° to 151.70(11)°. All moieties are connected by hydrogen bonds: d(O(5)–H(5)···N(1)#1) = 2.655(4) Å, d(O(1)–H(1B)···N(2)#2) = 2.776(5) Å, d(O(1)–H(1A)···O(6)#3) = 2.794(4) Å. Symmetry codes: #1 $-x, -y+1, -z+1$; #2 $-x+3/2, y-1/2, -z+1/2$; #3 $-x+3/2, y+1/2, -z+1/2$. These hydrogen bonds result in a 3D framework.

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