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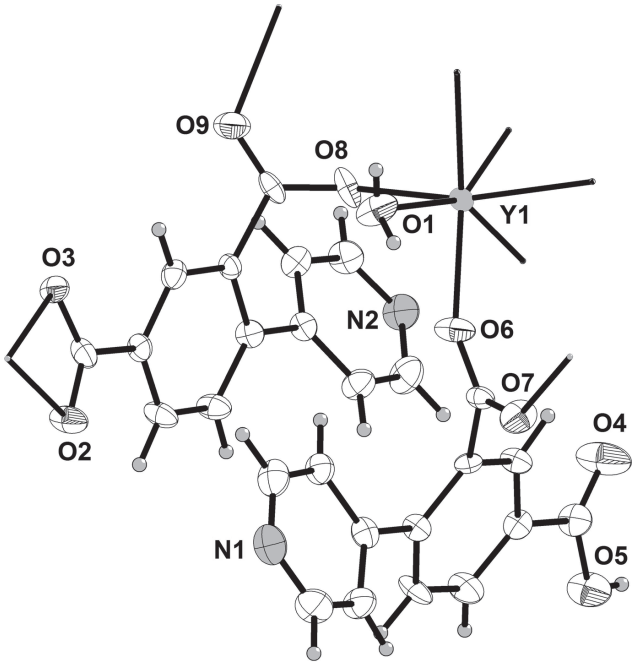
Crystal structure of poly[aqua-(μ$_3$-4-(pyridin-4-yl)isophthalato-κ^4*O*,*O*′:*O*″:*O*‴)-(μ$_2$-5-carboxy-2-(pyridin-4-yl)benzoato-κ^2*O*:*O*′)yttrium(III)], $C_{26}H_{17}N_2O_9Y$



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Abstract

$C_{26}H_{17}N_2O_9Y$, monoclinic, $P2_1/n$ (no. 14), $a = 8.9349(7)$ Å, $b = 9.3488(12)$ Å, $c = 28.1854(18)$ Å, $\beta = 95.061(7)°$, $V = 2345.2(4)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0496$, $wR_{ref}(F^2) = 0.1248$, $T = 293(2)$ 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.

Source of material

A mixture of $Y(NO_3)_3{\cdot}6H_2O$ (0.0434 g, 0.1 mmol), 4-(pyridin-4-yl)-isophthalic acid (0.1 mmol, 24.3 mg) and distilled water

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Table 1: Data collection and handling.

Crystal:	Block, colourless
Size:	0.41 × 0.35 × 0.29 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	2.55 cm^{-1}
Diffractometer, scan mode:	Multiwire detector, φ and ω-scans
$2\theta_{max}$, completeness:	25.5°, >95%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	9769, 4172, 0.046
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 2701
$N(param)_{refined}$:	344
Programs:	SHELX [1]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Y1	0.79209(5)	0.50175(7)	0.736845(15)	0.01955(16)
N1	0.1057(6)	0.0781(7)	0.66182(18)	0.0392(14)
N2	0.8388(6)	0.7563(7)	0.55853(17)	0.0384(14)
O1	0.5707(5)	0.4516(5)	0.77299(13)	0.0404(12)
H1W	0.5854	0.4813	0.7959	0.061*
H2W	0.5504	0.3630	0.7741	0.061*
O2	−0.0719(4)	0.4936(5)	0.66863(12)	0.0370(11)
O3	−0.0050(4)	0.6546(4)	0.72271(12)	0.0264(10)
O4	1.0082(6)	0.3217(7)	0.54000(16)	0.0670(18)
O5	0.9035(5)	0.1992(6)	0.47915(13)	0.0492(14)
H5	0.9847	0.2133	0.4684	0.074*
O6	0.6742(5)	0.3335(5)	0.69184(13)	0.0355(11)
O7	0.6629(5)	0.0978(5)	0.68947(12)	0.0383(12)
O8	0.6658(4)	0.6918(5)	0.70747(13)	0.0357(12)
O9	0.5153(5)	0.8579(5)	0.73112(13)	0.0381(12)
C1	0.7612(7)	0.2317(7)	0.54411(17)	0.0248(14)
C2	0.6264(7)	0.1964(7)	0.51867(18)	0.0339(17)
H2	0.6220	0.1888	0.4857	0.041*
C3	0.4982(7)	0.1724(7)	0.54175(17)	0.0324(16)
H3	0.4085	0.1501	0.5240	0.039*
C4	0.5020(6)	0.1814(6)	0.59163(16)	0.0227(14)
C5	0.6379(6)	0.2198(6)	0.61680(16)	0.0201(14)
C6	0.7633(6)	0.2481(7)	0.59331(16)	0.0250(14)
H6	0.8509	0.2786	0.6106	0.030*
C7	0.3644(6)	0.1486(7)	0.61584(17)	0.0258(14)
C8	0.2770(7)	0.0297(7)	0.6030(2)	0.0346(17)
H8	0.3018	−0.0281	0.5780	0.041*
C9	0.1537(7)	−0.0031(9)	0.6271(2)	0.0433(17)
H9	0.1008	−0.0863	0.6187	0.052*
C10	0.1873(7)	0.1948(8)	0.6727(2)	0.0382(18)
H10	0.1555	0.2550	0.6961	0.046*
C11	0.3153(6)	0.2329(7)	0.65172(18)	0.0293(15)

Table 2 (continued)

Atom	x	y	z	U_{iso}*/U_{eq}
H11	0.3683	0.3148	0.6617	0.035*
C12	0.9048(7)	0.2562(8)	0.52111(19)	0.0331(16)
C13	0.6582(6)	0.2178(7)	0.67050(17)	0.0223(13)
C14	0.7708(8)	0.6312(8)	0.5513(2)	0.0429(19)
H14	0.8120	0.5652	0.5315	0.051*
C15	0.6399(7)	0.5941(7)	0.57214(19)	0.0333(16)
H15	0.5957	0.5051	0.5661	0.040*
C16	0.5770(6)	0.6899(7)	0.60157(17)	0.0236(14)
C17	0.6454(7)	0.8226(7)	0.60778(19)	0.0290(15)
H17	0.6046	0.8920	0.6265	0.035*
C18	0.7755(7)	0.8509(8)	0.5858(2)	0.0353(16)
H18	0.8205	0.9401	0.5904	0.042*
C19	0.4359(6)	0.6571(6)	0.62422(17)	0.0231(14)
C20	0.3161(6)	0.5897(7)	0.59810(18)	0.0289(15)
H20	0.3273	0.5607	0.5670	0.035*
C21	0.1816(6)	0.5648(7)	0.61710(18)	0.0290(15)
H21	0.1048	0.5161	0.5995	0.035*
C22	0.1615(6)	0.6130(7)	0.66275(18)	0.0235(14)
C23	0.2785(6)	0.6814(7)	0.68890(18)	0.0253(14)
H23	0.2641	0.7151	0.7192	0.030*
C24	0.4159(6)	0.7008(6)	0.67122(17)	0.0203(13)
C25	0.0192(6)	0.5862(7)	0.68558(18)	0.0266(15)
C26	0.5411(6)	0.7568(7)	0.70510(18)	0.0245(14)

(10 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner at 443 K for 34 h, followed by slow cooling to room temperature. Colourless crystals of the compound formed.

Experimental details

H atoms were placed in calculated positions and were included in the refinement in the riding model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$ and $U_{iso}(H) = 1.5U_{eq}(O)$.

Discussion

Research on coordination complexes has made considerable progress in the fields of supramolecular chemistry and crystal engineering, owing to their intriguing architectures and functional applications, such as gas storage [2], catalysis [3], magnetism [4] and luminescence [5]. Studies in this field focus on the rational design of novel frameworks and the relationships between their structures and properties. 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 metal ions to form infinite network structures, such as chain structures and 2- or 3D networks [6]. 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, etc.

The asymmetric unit of the title structure contains one Y(III) metal center, one water molecule, one organic monoanion, and one organic dianion as bridging ligands to construct a coordination polymer. The yttrium atom is seven-coordinated by one water ligands, six oxygen atoms from two organic ligands (*cf*. the figure). The Y—O1 bond lengths is 2.350(4) Å, the Y—O6 bond lengths are 2.226(4) Å, the Y—O8 bond lengths are 2.225(4) Å. The bond angles of O—Y—O are in the range of 55.04(14)° to 161.53(16)°. All moieties are connected by hydrogen bonds d(O(5)—H(5)···N(2)#2) = 2.652(7) Å, d(O(1)—H(2W)···O(3)#3) = 2.844(6) Å, d(O(1)—H(1W)···O(7)#1) = 2.864(6) Å, d(O(1)—H(1W)···N(1)#4) =2.788(6) Å. Symmetry codes: #1 −x + 3/2, y + 1/2, −z + 3/2; #2 −x + 2, −y + 1, −z + 1; #3 −x + 1/2, y − 1/2, −z + 3/2; #4 −x + 1/2, y + 1/2, −z + 3/2.

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