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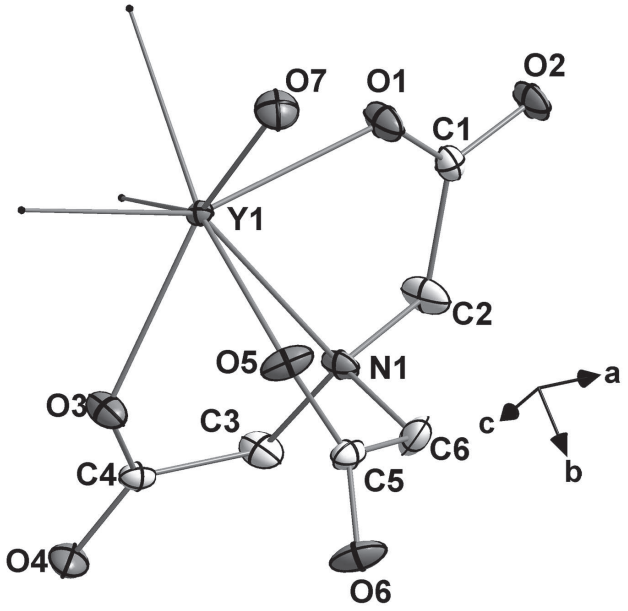
Crystal structure of poly[aqua(μ_4-2,2′,2″-nitrilotriacetato-κ^6*O*^{1},*O*^{3},*O*^{5}:*O*^{2}:*O*^{4}:*O*^{6})-yttrium(III)], $C_6H_8NO_7Y$



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Abstract

$C_6H_8NO_7Y$, monoclinic, $P2_1/n$ (no. 14), $a = 6.7457(7)$ Å, $b = 6.5637(6)$ Å, $c = 19.8466(19)$ Å, $\beta = 93.352(2)°$, $V = 877.24(15)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0245$, $wR_{ref}(F^2) = 0.0604$, $T = 296(2)$ K.

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A part 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.

Table 1: Data collection and handling.

Crystal:	Prism, colorless
Size:	0.20 × 0.04 × 0.04 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	6.67 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, ω-scans
θ_{max}, completeness:	28.3°, >98%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	5577, 2145, 0.024
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1898
$N(param)_{refined}$:	136
Programs:	Bruker programs [1], SHELX [2]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Y1	0.23106(3)	0.73376(3)	0.10466(2)	0.00715(8)
N1	0.4927(3)	0.9840(3)	0.15820(10)	0.0126(4)
C1	0.7126(3)	0.7420(3)	0.10219(11)	0.0126(5)
C2	0.6952(4)	0.9002(4)	0.15684(13)	0.0209(5)
H2A	0.732133	0.839184	0.200292	0.025*
H2B	0.787475	1.010314	0.149557	0.025*
C3	0.4467(4)	1.0286(4)	0.22867(12)	0.0180(5)
H3A	0.495077	1.163724	0.240738	0.022*
H3B	0.515681	0.931604	0.258534	0.022*
C4	0.2268(3)	1.0180(3)	0.23872(11)	0.0119(5)
C5	0.2723(4)	1.2106(3)	0.08531(12)	0.0131(5)
C6	0.4786(4)	1.1719(4)	0.11658(14)	0.0199(5)
H6A	0.570409	1.161458	0.080918	0.024*
H6B	0.518800	1.287518	0.144607	0.024*
O1	0.5566(2)	0.6790(3)	0.07198(9)	0.0189(4)
O2	0.8845(2)	0.6769(3)	0.09225(9)	0.0174(4)
O3	0.1163(2)	0.9421(2)	0.19264(8)	0.0158(4)
O4	0.1672(3)	1.0788(3)	0.29428(8)	0.0190(4)
O5	0.1767(3)	1.0592(2)	0.06139(8)	0.0179(4)
O6	0.2069(3)	1.3881(3)	0.08213(9)	0.0226(4)
O7	0.1764(3)	0.7069(3)	−0.01379(8)	0.0179(4)
H7A	0.070426	0.771065	−0.034165	0.022*
H7B	0.177026	0.588175	−0.033075	0.022*

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Source of material

The source materials, nitrilotriacetic acid (H_3NTA), yttrium nitrate hexahydrate and sodium carbonate were purchased

from Jinan Camolai Trading. All chemicals of analytical grade were obtained from commercial sources and used without further purification. A mixture of H_3NTA (0.10 g), $Y(NO_3)_3 \cdot 6H_2O$ (0.03 g), Na_2CO_3 (0.05 g) and deionized water (15 mL) was placed in a 30 mL Teflon-lined stainless steel autoclave. The autoclave was heated to 180 °C under autogenously pressure for 72 h. After being cooled to room temperature at a rate of 10 °C/h, colorless prismatic crystals were recovered by filtration, washed with distilled water and air dried.

Experimental details

The H atoms of C atoms were positioned geometrically and refined with a riding model, with C—H = 0.97 Å and $U_{iso}(H) = 1.2\,U_{eq}(C)$. The H atoms of water and carboxyl were located in difference Fourier maps, and then refined with a riding model, with $U_{iso}(H) = 1.2U_{eq}(O)$.

Discussion

The design and construction of coordination polymers (CPs) has been one of the most active areas of material research in recent years. Being easily and efficiently synthesized from relatively simple subunits, CPs exhibit fascinating variety of topologies but also wing to their potential applications as functional materials [3–5]. Most of CPs are usually made by combining a organic network with an inorganic component. The selection of suitable organic ligands is crucial for constructing extended coordination frameworks. As one of the most fascinating ligands, NTA^{3-} is selected because it can afford six O and one N as donor atoms to coordinate with various metals to assemble supramolecular structures. Among them, several structures have been reported with metal-NTA networks involving rare-earth metal ions, including $[Eu(NTA)(H_2O)_2]_n \cdot H_2O$ and $[Ln(NTA)(H_2O)]_n$ (Ln = La, Pr, Nd, Sm, Eu, Gd, Tb, Ho, Er and Tm) [6–11]. In order to enrich this family of compounds, we report the synthesis and crystal structure of $[Y(NTA)(H_2O)]_n$.

X-ray single crystal X-ray diffraction (SC-XRD) analysis reveals that compound $[Y(NTA)(H_2O)]_n$ exhibits a two-dimensional (2D) structure that is constructed by deprotonated NTA^{3-} ligands and Y^{3+} ions, as shown in the figure. There is one Y^{3+} ion, one fully deprotonated NTA^{3-} ligand and one coordinated aqua in the asymmetric unit. Each Y^{3+} is surrounded by seven O atoms and one N atom in a distorted dodecahedron. In this coordination scheme, three O atoms and N atom come from a single NTA^{3-} ligand, three O atoms belongs to three other NTA^{3-} ligands, and one O atom belongs to a coordinated water molecule. The Y—O bond distances fall in the range of 2.3165(17)–2.3825(16) Å and the Y—N bond distance is 2.5932(19) Å, which are typical cor related Y^{3+} compounds [12, 13]. Moreover, the rationality of eight Y—O(N) bonds can be evaluated by bond valance sum (BVS) calculation [14]. The BVS for Y^{3+} is 3.216, and close to 3.0. Adjacent layers are interconnected by hydrogen bonds to generate the final three dimensional structure of the title compound.

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