Qiu-Xia Liu and Guan-Feng Li*

Crystal structure of poly[μ_2 -acetato- κ^3 -O,O':O') diaqua(μ_3 -isophthalato- κ^4 O,O':O'':O''') yttrium(III)] monohydrate, $C_{20}H_{24}O_{17}Y_2$

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.45 × 0.32 × 0.24 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	45.8 cm ⁻¹
Diffractometer, scan mode:	Broker APEX-II, φ and ω
$2\theta_{\max}$, completeness:	51°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	6019, 2375, 0.026
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1908
$N(\text{param})_{\text{refined}}$:	182
Programs:	Broker programs [1], SHELX [2]

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Abstract

$C_{20}H_{24}O_{17}Y_2$, monoclinic, $P2_1/c$ (no. 14), $a = 10.347(2)$ Å, $b = 12.314(3)$ Å, $c = 10.090(2)$ Å, $\beta = 93.967(3)^\circ$, $V = 1282.5(5)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0292$, $wR_{\text{ref}}(F^2) = 0.0579$, $T = 296(2)$ K.

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The asymmetric unit of the title crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method 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), isophthalic acid (0.1 mmol, 0.0167 g), CH_3COOH (1 mL) and distilled water (10 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner at 413 K for 48 h, followed by slow cooling

to room temperature. Colourless crystals of the compound were formed.

Experimental details

All H atoms were positioned geometrically (O–H = 0.83 Å and C–H = 0.93 or 0.96 Å) and refined using a riding model, with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$ and $1.5U_{\text{eq}}(C_{\text{methyl}}, O)$.

Comment

In recent years, research on coordination complexes has been closely linked to the fields of supramolecular chemistry and crystal engineering. Coordination complexes have found applications in the fields of gas storage [3], catalysis [4], magnetism [5] and luminescence [6]. The rational design and synthesis of novel structural frameworks and the relationships between their structures and properties is an area of intense research activity. 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 one-dimensional (1D) chain structures and 2- or 3-D networks [7]. 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, $\pi \cdots \pi$ stacking, and host-guest ionic interactions [8].

The asymmetric unit of the title structure contains one Y(III) ion, two coordinated water molecules, one half of a solvent water molecule, one acetate ion and one

*Corresponding author: Guan-Feng Li, College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471022, Henan Province, P. R. China, e-mail: shihui471022@126.com

Qiu-Xia Liu: College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471022, Henan Province, P. R. China

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

Atom	x	y	z	U _{iso} ^a /U _{eq}
Y1	0.62757(3)	−0.14040(2)	−0.00463(3)	0.01505(10)
O1 ^a	0.5972(7)	0.5077(5)	0.0930(6)	0.0639(19)
H5W ^a	0.6025	0.5265	0.1715	0.096*
H6W ^a	0.5626	0.4478	0.0762	0.096*
O2	0.4828(2)	−0.1344(2)	−0.1940(2)	0.0362(6)
H1W	0.4260	−0.0862	−0.2014	0.054*
H2W	0.4643	−0.1828	−0.2492	0.054*
O3	0.5856(3)	−0.3266(2)	−0.0865(2)	0.0360(6)
H3W	0.6244	−0.3550	−0.1468	0.054*
H4W	0.6136	−0.3659	−0.0245	0.054*
O4	0.5963(2)	0.04312(19)	−0.0625(2)	0.0278(6)
O5	0.5498(2)	0.20939(19)	−0.1161(2)	0.0263(5)
O6	0.6725(2)	−0.04256(18)	0.2072(2)	0.0211(5)
O7	0.8304(2)	−0.0533(2)	0.0730(2)	0.0291(6)
O8	1.2308(2)	0.1622(2)	0.1652(2)	0.0310(6)
O9	1.2735(2)	0.23537(19)	0.3629(2)	0.0283(6)
C1	0.7895(3)	−0.0197(3)	0.1790(3)	0.0205(7)
C2	0.8731(3)	0.0474(3)	0.2726(3)	0.0219(7)
C3	0.8347(4)	0.0739(3)	0.3982(3)	0.0391(10)
H3	0.7553	0.0496	0.4243	0.047*
C4	0.9133(4)	0.1355(4)	0.4836(4)	0.0540(13)
H4	0.8872	0.1521	0.5676	0.065*
C5	1.0313(4)	0.1731(3)	0.4452(3)	0.0386(10)
H5	1.0836	0.2156	0.5032	0.046*
C6	1.0717(3)	0.1474(3)	0.3205(3)	0.0212(7)
C7	0.9921(3)	0.0846(3)	0.2342(3)	0.0207(7)
H7	1.0184	0.0674	0.1505	0.025*
C8	1.2008(3)	0.1849(3)	0.2798(3)	0.0177(7)
C9	0.6246(3)	0.1293(3)	−0.1193(3)	0.0242(8)
C10	0.7460(5)	0.1361(4)	−0.1895(6)	0.087(2)
H10A	0.8181	0.1145	−0.1303	0.131*
H10B	0.7586	0.2094	−0.2183	0.131*
H10C	0.7399	0.0887	−0.2652	0.131*

^aOccupancy: 0.5.

isophthalate dianion as bridging ligands to construct a new coordination polymer. Each yttrium cation is nine-coordinated in a distorted polyhedron manner and the two oxygen atoms (O6 and O7) from isophthalate ligands show Y–O bond lengths of 2.470(2) Å and 2.437(2) Å, respectively. The oxygen atom O4 and O5 belonging to the bridging acetate ligand are coordinated with Y–O distances of 2.351(2) and 2.426(2) Å. The Y–O distances of the two oxygen atoms (O2

and O3) from coordinated water molecules are 2.347(2) Å and 2.466(2) Å, respectively. The bond angles of O–Y–O are in the range of 49.12(7)° to 149.73(9)°. In addition, there are intermolecular hydrogen bonds between coordinated and uncoordinated water molecules $d(\text{O}(1)–\text{H}(5\text{W})\cdots\text{O}(2)\#9) = 2.967(6)$ Å, $d(\text{O}(1)–\text{H}(6\text{W})\cdots\text{O}(3)\#3) = 2.925(11)$ Å, $d(\text{O}(3)–\text{H}(4\text{W})\cdots\text{O}(1)\#6) = 2.725(6)$ Å. Coordinated and uncoordinated water molecules are also connected with adjacent isophthalate and acetate ligands by intermolecular hydrogen bonds $d(\text{O}(2)–\text{H}(1\text{W})\cdots\text{O}(6)\#3) = 2.705(3)$ Å, $d(\text{O}(3)–\text{H}(3\text{W})\cdots\text{O}(6)\#7) = 2.827(3)$ Å, $d(\text{O}(3)–\text{H}(4\text{W})\cdots\text{O}(9)\#2) = 2.710(3)$ Å. Coordinated water molecules are directly connected via intermolecular hydrogen bonds $d(\text{O}(2)–\text{H}(2\text{W})\cdots\text{O}(5)\#8) = 2.719(3)$ Å. Symmetry codes: #2 $-x+2$, $y-1/2$, $-z+1/2$; #3 $-x+1$, $-y$, $-z$; #6 x , $y-1$, z ; #7 x , $-y-1/2$, $z-1/2$; #8 $-x+1$, $y-1/2$, $-z-1/2$; #9 x , $-y+1/2$, $z+1/2$. All these intermolecular contacts result in a 3D framework.

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