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Crystal structure of diaqua-(acetato- $\kappa^3 O, O':O''$)-(μ_3 -4,6-di(1*H*-imidazol-1-yl)isophthalato- $\kappa^4 O:O':O'', O'''$)lanthanum(III), $C_{16}H_{15}LaN_4O_8$

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.20 × 0.18 × 0.16 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	2.36 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω -scans
$\theta_{\max}$, completeness:	25°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	9838, 3247, 0.038
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2896
$N(\text{param})_{\text{refined}}$:	263
Programs:	CrysAlis ^{PRO} [1], SHELX [2]

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
LA1	0.28957(2)	0.22173(2)	0.32527(2)	0.01701(11)
O1	0.4287(3)	0.16423(18)	0.2311(3)	0.0369(8)
O2	0.4427(3)	0.23978(18)	0.0399(3)	0.0337(8)
O3	0.6283(2)	−0.12579(16)	0.2237(3)	0.0253(7)
O6	0.2109(2)	0.09302(18)	0.1587(3)	0.0329(8)
H6A	0.250984	0.080557	0.107839	0.049*
H6B	0.206854	0.049817	0.211519	0.049*
O4	0.7486(2)	−0.12053(16)	0.1100(3)	0.0262(7)
O5	0.3296(3)	0.08962(17)	0.4794(3)	0.0439(9)
H5B	0.340824	0.103359	0.569172	0.066*
H5A	0.276424	0.055549	0.451221	0.066*
C8	0.6397(4)	0.4188(3)	0.2250(6)	0.0459(14)
H8	0.619812	0.466969	0.268213	0.055*
N2	0.6862(4)	0.4222(2)	0.1142(5)	0.0465(11)
N1	0.6672(3)	0.28645(19)	0.1735(4)	0.0251(9)
N3	0.8780(3)	0.0274(2)	0.2101(4)	0.0272(8)
N4	1.0366(3)	0.0062(3)	0.1856(5)	0.0474(11)
C14	0.4758(3)	0.1862(2)	0.1435(4)	0.0248(10)
C12	0.9326(4)	−0.0280(3)	0.3198(5)	0.0511(14)
H12	0.908015	−0.052265	0.391713	0.061*
C10	0.9457(4)	0.0451(3)	0.1343(5)	0.0413(12)
H10	0.928531	0.081711	0.052911	0.050*
C6	0.6719(4)	0.1943(3)	0.1720(4)	0.0206(9)
C3	0.6873(3)	0.0138(2)	0.1770(4)	0.0193(9)
C2	0.5927(3)	0.0553(2)	0.1702(4)	0.0191(9)
H2	0.534354	0.022006	0.170961	0.023*
C4	0.7757(3)	0.0644(2)	0.1877(4)	0.0223(9)
C1	0.5820(3)	0.1453(2)	0.1623(4)	0.0188(9)
C13	0.6881(3)	−0.0839(2)	0.1711(4)	0.0199(9)
C11	1.0285(4)	−0.0404(4)	0.3035(6)	0.0572(15)

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Abstract

$C_{16}H_{15}LaN_4O_8$, monoclinic, $P2_1/c$ (no. 14), $a = 13.2370(6)$ Å, $b = 15.4658(5)$ Å, $c = 9.5723(4)$ Å, $\beta = 108.834(4)^\circ$, $V = 1854.72(14)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0342$, $wR_{\text{ref}}(F^2) = 0.0814$, $T = 293(2)$ K.

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The crystal structure is shown in the figure ($' = x$, $0.5 - y$, $0.5 + y$; $'' = 1 - x$, $0.5 + y$, $0.5 - z$). 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}
H11	1.081944	−0.075586	0.363679	0.069*
C5	0.7688(3)	0.1535(2)	0.1863(4)	0.0247(10)
H5	0.829189	0.186634	0.194812	0.030*
C7	0.6275(4)	0.3369(3)	0.2612(5)	0.0366(12)
H7	0.597889	0.318009	0.331764	0.044*
C9	0.7022(4)	0.3412(3)	0.0879(5)	0.0377(12)
H9	0.733768	0.323252	0.018958	0.045*
O7	0.1014(3)	0.21291(19)	0.3288(3)	0.0410(9)
O8	0.1984(3)	0.22760(15)	0.5621(3)	0.0285(7)
C16	0.0051(5)	0.2397(5)	0.4905(6)	0.0724(19)
H16A	0.018922	0.255063	0.592099	0.109*
H16B	−0.036457	0.187632	0.468897	0.109*
H16C	−0.033502	0.285610	0.428419	0.109*
C15	0.1101(4)	0.2253(2)	0.4619(5)	0.0300(11)

Source of materials

H₂L (0.0090 g, 0.03 mmol), and La(CH₃COO)₃ (0.0095 g, 0.03 mmol) were dissolved in distilled water (8 mL). The resultant solution was allowed to evaporate slowly at room temperature. Yellow block single crystals were obtained.

Experimental details

Absorption corrections were applied by using multi-scan program. The structure was refined based on *F*² with the SHELXL [2] software package. Hydrogen atoms attached to C of the title complex located in difference electron density maps, and treated as riding atoms. The *U*_{iso} values of the hydrogen atoms were set to 1.2*U*_{eq}(C).

Comment

The construction of metal-containing supramolecular networks has been an active field [3–7]. Coordinate covalent bonding [4] and noncovalent interactions (hydrogen bonding) [5–7] are two well established essentials crystal engineering. Recently, several groups have utilized hydrogen bonding interactions to construct new, porous materials with permanent porosity and highly selective gas separation [8, 9]. We, aim to construct intriguing architectures through coordinative and hydrogen bonding interactions. Thus, we selected a carboxylate ligand.

The asymmetric unit contains one La³⁺ ion, one fully protonated dicarboxylate ligand, two coordinated water molecules and one coordinated acetate anion. Adjacent carboxylate ligands generate infinite chain via bridging acetic group chelating carboxylic group (O1–O2). Such chains linked through another chelating carboxylic group (O3–O4) to give rise to layered structure, which further linked through O–H···N hydrogen bonds (O6···N4, 2.752(5) Å) to give rise to three-dimensional network.

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