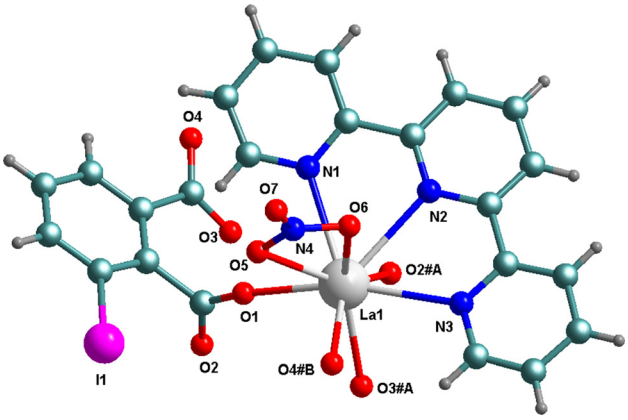
Bin Cai* and Yuning Meng

The crystal structure of catena-[nitrato-κ^2O, O'-(μ_3-3-iodobenzene-1,2-dicarboxylato-κ^4O:O': O'',O''')-(2,2′:6′,2″-terpyridine-κ^3N,N', N'')lanthanum(III)], $C_{23}H_{14}IN_4O_7La$



https://doi.org/10.1515/ncrs-2023-0036
Received January 22, 2023; accepted March 5, 2023;
published online March 16, 2023

Abstract

$C_{23}H_{14}IN_4O_7La$, triclinic, $P\bar{1}$ (no. 2), a = 8.2438(3) Å, b = 12.3786(5) Å, c = 12.6230(5) Å, α = 111.802(1)°, β = 91.144(1)°, γ = 100.6470(10)°, V = 1169.86(8) Å^3, Z = 2, $R_{gt}(F)$ = 0.0313, w$R_{ref}(F^2)$ = 0.1051, T = 296 K.

CCDC no.: 2246341

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.25 × 0.20 × 0.15 mm
Wavelength:	Mo *Kα* radiation (0.71073 Å)
μ:	3.20 mm^{-1}
Diffractometer, scan mode:	φ and ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	28,225, 4123, 0.052
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 3535
$N(param)_{refined}$:	325
Programs:	Bruker [1], Olex2 [2], Shelx [3, 4]

1 Source of materials

The educts 0.433 g lanthanum hexahydrate (1 mmol), 0.292 g (1 mmol) 3-iodobenzene-1,2-dicarboxylic acid, 0.233 g 2,2′:6′,2″-terpyridine (1 mmol), and 0.080 g NaOH (2 mmol) were mixed with 8 mL H_2O, then added to a 25 mL Teflon-lined stainless steel autoclave at 413 K for 72 h. Many colourless block crystals were separated, washed with distilled water and anhydrous ethanol, then dried in air. Yield: 66% (based on 3-iodobenzene-1,2-dicarboxylic acid).

2 Experimental details

The structure was solved by direct methods with the Shelxs-2018 program. All H-atoms from C and N atoms were positioned with idealized geometry (U_{iso}(H) = 1.2U_{eq}(C)) using a riding model with C–H = 0.93 Å.

3 Comment

Although benzenedicarboxylic acid, including benzene-1,2-, 1,3- and 1,4-dicarboxylic acids and 2,2′:6′,2″-terpyridine or their derivatives have been used as co-ligands to construct some lanthanide complexes [5–11], to the best of our knowledge, there has not been reported any result of lanthanide complex based on 3-iodobenzene-1,2-dicarboxylic acid and 2,2′:6′,2″-terpyridine.

As shown in the figure, the asymmetrical unit is made of one La(III) cation, one 3-iodobenzene-1,2-dicarboxylate

***Corresponding author: Bin Cai**, College of Materials and Chemical Engineering, Henan University of Urban Construction, Pingdingshan 467036, Henan, P. R. China, E-mail: caib@hncj.edu.cn. https://orcid.org/0000-0002-3573-5651
Yuning Meng, College of Materials and Chemical Engineering, Henan University of Urban Construction, Pingdingshan 467036, Henan, P. R. China

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4184 (7)	0.6668 (6)	0.2866 (5)	0.0339 (14)
H1	0.471366	0.720550	0.357220	0.041*
C2	0.2912 (7)	0.6960 (6)	0.2386 (6)	0.0385 (15)
H2	0.255416	0.766018	0.277999	0.046*
C3	0.2181 (8)	0.6218 (6)	0.1332 (6)	0.0427 (16)
H3	0.134074	0.641176	0.097883	0.051*
C4	0.2707 (7)	0.5167 (6)	0.0792 (5)	0.0408 (16)
H4	0.222502	0.464385	0.006707	0.049*
C5	0.3952 (7)	0.4901 (5)	0.1334 (5)	0.0317 (14)
C6	0.4517 (7)	0.3767 (5)	0.0797 (5)	0.0311 (13)
C7	0.3598 (9)	0.2852 (6)	−0.0151 (6)	0.0509 (19)
H7	0.262806	0.294611	−0.046345	0.061*
C8	0.4139 (9)	0.1813 (7)	−0.0617 (6)	0.061 (2)
H8	0.352463	0.118190	−0.123854	0.073*
C9	0.5593 (9)	0.1707 (6)	−0.0161 (6)	0.0526 (19)
H9	0.597574	0.100315	−0.047283	0.063*
C10	0.6485 (7)	0.2644 (5)	0.0759 (5)	0.0334 (14)
C11	0.8129 (7)	0.2616 (5)	0.1231 (5)	0.0331 (14)
C12	0.8972 (9)	0.1741 (7)	0.0634 (7)	0.060 (2)
H12	0.850296	0.114823	−0.006305	0.072*
C13	1.0528 (10)	0.1761 (7)	0.1091 (7)	0.068 (3)
H13	1.110703	0.117448	0.070951	0.082*
C14	1.1192 (8)	0.2643 (6)	0.2096 (6)	0.0478 (18)
H14	1.223650	0.267667	0.241457	0.057*
C15	1.0306 (7)	0.3477 (5)	0.2630 (5)	0.0376 (15)
H15	1.077449	0.408149	0.332131	0.045*
C16	0.5014 (6)	0.6860 (5)	0.5815 (5)	0.0239 (12)
C17	0.4106 (7)	0.7848 (5)	0.5848 (4)	0.0236 (12)
C18	0.4925 (7)	0.9028 (5)	0.6277 (5)	0.0323 (14)
C19	0.4116 (8)	0.9930 (5)	0.6333 (6)	0.0455 (17)
H19	0.468649	1.071721	0.664711	0.055*
C20	0.2478 (8)	0.9666 (6)	0.5926 (6)	0.0454 (17)
H20	0.193053	1.027137	0.596525	0.054*
C21	0.1653 (7)	0.8497 (5)	0.5460 (5)	0.0373 (15)
H21	0.054968	0.831487	0.516583	0.045*
C22	0.2430 (6)	0.7590 (5)	0.5419 (5)	0.0251 (12)
C23	0.1478 (7)	0.6325 (5)	0.4868 (5)	0.0251 (12)
I1	0.74624 (5)	0.95341 (4)	0.68699 (4)	0.04903 (17)
La1	0.72448 (4)	0.52213 (3)	0.34616 (3)	0.02114 (13)
N1	0.4705 (6)	0.5647 (4)	0.2372 (4)	0.0308 (11)
N2	0.5949 (6)	0.3674 (4)	0.1253 (4)	0.0274 (11)
N3	0.8796 (6)	0.3482 (4)	0.2223 (4)	0.0315 (11)
N4	0.8609 (6)	0.7189 (4)	0.2585 (4)	0.0316 (12)
O1	0.5876 (5)	0.6507 (3)	0.4998 (3)	0.0316 (9)
O2	0.4874 (4)	0.6512 (3)	0.6624 (3)	0.0271 (9)
O3	0.2016 (4)	0.5524 (3)	0.5053 (3)	0.0286 (9)
O4	0.0159 (5)	0.6146 (4)	0.4242 (4)	0.0347 (10)
O5	0.7996 (5)	0.7445 (4)	0.3518 (4)	0.0374 (10)
O6	0.8524 (5)	0.6091 (4)	0.1995 (3)	0.0378 (10)
O7	0.9275 (6)	0.7936 (4)	0.2232 (4)	0.0512 (12)

anion, one 2,2′:6′,2″-terpyridine and one nitrate. The La(III) cation is nine-coordinated by four oxygen atoms (O1, O2#A, O3#A and O4#B, code #A: $1-x, 1-y, 1-z$; code #B: $1+x, y, z$) from three completely deprotonated μ_3-iodobenzene-1,2-dicarboxylate anions, two oxygen atoms from one μ_2-nitrate (O5 and O6), and three nitrogen atoms (N1, N2 and N3) from one 2,2′:6′,2″-terpyridine. The neighbouring La(III) cations are linked by μ_3-iodobenzene-1,2-dicarboxylate anions to generate chain structure, further connected by nonclassical hydrogen bonds C4–H4H7···O6, C7–H7···O7 and C20–H20H7···O5, with HH7···A distances 2.460, 2.440 and 2.643 Å, respectively. All of the bond lengths are similar to the reported results [5–11].

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

References

1. Bruker. *SAINT v8.40A*; Bruker AXS Inc: Madison, Wisconsin, USA, 2016.
2. Bourhis L. J., Dolomanov O. V., Gildea R. J., Howard J. A. K., Puschmann H. The anatomy of a comprehensive constrained, restrained refinement program for the modern computing environment–Olex2 dissected. *Acta Crystallogr.* 2015, *A71*, 59–75.
3. Sheldrick G. M. Crystal structure refinement with Shelxl. *Acta Crystallogr.* 2015, *C71*, 3–8.
4. Sheldrick G. Using phases to determine the space group. *Acta Crystallogr.* 2018, *A74*, a353.
5. Hu Y.-C., Bai C., Hu H.-M., Li C.-T., Zhang T.-H., Liu W. Lanthanide coordination polymers based on designed bifunctional 2-(2,2′:6′,2″-terpyridin-4′-yl)benzenesulfonate ligand: syntheses, structural diversity and highly tunable emission. *Acta Crystallogr.* 2019, *B75*, 855–864.
6. Bai C., Li C.-T., Hu H.-M., Liu B., Li J.-D., Xue G. Dy(iii) zig-zag chains assembled in a 3D framework with single-molecule magnet behaviour. *Dalton Trans.* 2019, *48*, 814–817.
7. Bai C., Liu B., Hu H.-M., Li J.-D., Wang X., Xue G. Structural investigation of one- and three-dimensional lanthanide(III) coordination polymers based on functionalized terpyridine carboxylate and aromatic dicarboxylate ligands. *Acta Crystallogr.* 2019, *C75*, 422–432.
8. Wei Y., Li Q., Sa R., Wu K. A white-light-emitting LnMOF with color properties improved via Eu^{3+} doping: an alternative approach to a rational design for solid-state lighting. *Chem. Commun.* 2014, *50*, 1820–1823.
9. Zheng Z., Lu H., Wang Y., Bao H., Li Z.-J., Xiao G.-P., Lin J., Qian Y., Wang J.-Q. Tuning of the network dimensionality and photoluminescent properties in homo- and heteroleptic lanthanide coordination polymers. *Inorg. Chem.* 2021, *60*, 1359–1366.
10. Wei Y., Sa R., Li Q., Wu K. Highly stable and sensitive LnMOF ratiometric thermometers constructed with mixed ligands. *Dalton Trans.* 2015, *44*, 3067–3074.
11. Du C.-J., Wang Z.-D., Zhu D.-F., Zhu Y.-L., Zeng Y. Crystal structure of 3-iodophthalic acid, $C_8H_5IO_4$. *Z. Kristallogr. N. Cryst. Struct.* 2020, *235*, 243–244.