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Crystal structure of *catena*-poly[(μ_2 -5-(*tert*-butyl)isophthalato- $\kappa^4 O, O': O'', O'''$)(-4'-(pyridin-4-yl)-2,2':6',2''-terpyridine- $\kappa^3 N, N', N''$)manganese(II)], $C_{32}H_{28}N_4O_5Mn$

Table 1: Data collection and handling.

Crystal:	Block, clear light colourless
Size:	0.21 × 0.18 × 0.18 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.54 mm ⁻¹
Diffractometer, scan mode:	Bruker SMART, φ and ω -scans
$\theta_{\max}$, completeness:	26°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	14833, 5266, 0.052
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 3374
$N(\text{param})_{\text{refined}}$:	385
Programs:	Bruker [1], SHELX [2], OLEX2 [3]

<https://doi.org/10.1515/ncrs-2018-0189>

Received May 29, 2018; accepted July 9, 2018; available online July 23, 2018

Abstract

$C_{32}H_{28}N_4O_5Mn$, monoclinic, $P2_1/c$ (no. 14), $a = 8.777(3)$ Å, $b = 30.975(11)$ Å, $c = 10.229(4)$ Å, $\beta = 105.412(7)^\circ$, $V = 2680.9(16)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0448$, $wR_{\text{ref}}(F^2) = 0.1136$, $T = 296(2)$ K.

CCDC no.: 1854556

The crystal structure is shown in the figure. Hydrogen atoms are omitted for clarity (symmetry code #1: $x, y, -1+z$). Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of 5-(*tert*-butyl)isophthalic acid (H_2tbp , 23 mg, 0.1 mmol), 4'-(pyridin-4-yl)-2,2':6',2''-terpyridine (PYTPY, 32 mg, 0.1 mmol), $Mn(OAc)_2 \cdot 4H_2O$ (25 mg, 0.1 mmol) and H_2O (12 mL) was stirred for 30 min, and the pH value of the solution was adjusted to about 6 with 1 M KOH. Then the mixture was transferred to a 25 mL Teflon-lined stainless

steel vessel and heated at 140 °C for 4 days, and then cooled to room temperature over 60 h. Colorless block crystals of 1 were obtained. Anal. (%) Calcd. for $C_{32}H_{28}MnN_4O_5$: C, 63.69, H 4.68, N 9.28. Found: C 63.74, H 4.62, N 9.31. IR (cm⁻¹): 3127 m, 2958 m, 1601 m, 1565 m, 1531 s, 1459 m, 1342 s, 1092 s, 885 s, 736 s.

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

Discussion

In recent years, a great deal of attention has focused on the self-assembly by metal-ligand interaction owing to luminescence, heterogeneous catalysis, gas storage/separations, and magnetic and electronic applications [4–7]. Although a lot of coordination polymers have been synthesized and characterized, precision synthesis of targeted structures has still been difficult [8, 9]. Among the plenty of ligands employed in the fabrication of coordination polymers, the multidentate *N*- and/or *O*-donor building blocks have received extensive attention [10]. For example, isophthalate and its derivatives with specific conformations and versatile coordination fashions can bind metal centers of specific coordination geometry to construct coordination polymers [11]. It is well known that the *N*-heterocyclic pyridine based organic molecules are also excellent ligands [12]. As an important polypyridyl ligand, 4'-(4-pyridyl)-2,2':6',2''-terpyridine (PYTPY) has been widely used to build supramolecular architectures because of its excellent coordinating ability and large conjugated system that may provide potential supramolecular recognition sites.

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
Mn1	0.32956(4)	0.34435(2)	0.25870(4)	0.02996(14)
O1	0.3152(3)	0.38997(6)	0.40596(19)	0.0527(6)
O2	0.2879(3)	0.32899(6)	0.50268(19)	0.0580(6)
O3	0.3746(3)	0.32855(6)	1.0055(2)	0.0645(7)
O4	0.3422(2)	0.38833(6)	1.10730(18)	0.0457(5)
N1	0.0772(2)	0.32335(6)	0.1787(2)	0.0317(5)
N2	0.3260(2)	0.27326(6)	0.25449(19)	0.0277(5)
N3	0.5802(2)	0.32102(6)	0.3354(2)	0.0327(5)
N4	0.3043(3)	0.04529(7)	0.2535(3)	0.0548(7)
C1	−0.0435(3)	0.35075(8)	0.1414(3)	0.0373(7)
H1	−0.0233	0.3802	0.1520	0.045*
C2	−0.1962(3)	0.33741(9)	0.0882(3)	0.0419(7)
H2	−0.2777	0.3575	0.0634	0.050*
C3	−0.2271(3)	0.29419(9)	0.0720(3)	0.0395(7)
H3	−0.3299	0.2844	0.0357	0.047*
C4	−0.1034(3)	0.26518(8)	0.1104(3)	0.0377(7)
H4	−0.1216	0.2356	0.0997	0.045*
C5	0.0471(3)	0.28071(8)	0.1648(2)	0.0295(6)
C6	0.1886(3)	0.25213(8)	0.2100(2)	0.0295(6)
C7	0.1818(3)	0.20785(8)	0.2095(2)	0.0333(7)
H7	0.0848	0.1939	0.1805	0.040*
C8	0.3196(3)	0.18380(8)	0.2520(3)	0.0321(6)
C9	0.4619(3)	0.20636(8)	0.2954(3)	0.0341(7)
H9	0.5572	0.1915	0.3230	0.041*
C10	0.4599(3)	0.25078(8)	0.2969(2)	0.0284(6)
C11	0.6053(3)	0.27809(8)	0.3439(2)	0.0284(6)
C12	0.7541(3)	0.26100(8)	0.3957(3)	0.0381(7)
H12	0.7690	0.2313	0.4022	0.046*
C13	0.8806(3)	0.28876(9)	0.4380(3)	0.0416(7)
H13	0.9818	0.2778	0.4739	0.050*
C14	0.8565(3)	0.33236(9)	0.4269(3)	0.0425(7)
H14	0.9405	0.3516	0.4536	0.051*
C15	0.7050(3)	0.34694(8)	0.3754(3)	0.0378(7)
H15	0.6883	0.3766	0.3679	0.045*
C16	0.3164(3)	0.13605(8)	0.2522(3)	0.0333(6)
C17	0.4337(3)	0.11136(9)	0.3376(3)	0.0432(8)
H17	0.5202	0.1247	0.3964	0.052*
C18	0.4209(4)	0.06732(9)	0.3346(3)	0.0549(9)
H18	0.5002	0.0517	0.3942	0.066*
C19	0.1942(4)	0.06897(9)	0.1717(3)	0.0535(9)
H19	0.1106	0.0546	0.1127	0.064*
C20	0.1943(3)	0.11315(8)	0.1674(3)	0.0420(7)
H20	0.1122	0.1277	0.1075	0.050*
C21	0.2988(3)	0.36866(9)	0.5055(3)	0.0354(7)
C22	0.2978(3)	0.39241(8)	0.6334(3)	0.0311(6)
C23	0.3207(3)	0.37020(8)	0.7539(2)	0.0315(6)
H23	0.3281	0.3402	0.7545	0.038*
C24	0.3328(3)	0.39225(8)	0.8740(2)	0.0301(6)
C25	0.3202(3)	0.43703(7)	0.8709(3)	0.0316(6)
H25	0.3270	0.4518	0.9514	0.038*
C26	0.2978(3)	0.46025(8)	0.7518(2)	0.0303(6)
C27	0.2867(3)	0.43691(8)	0.6334(3)	0.0346(7)
H27	0.2713	0.4517	0.5518	0.042*
C28	0.3519(3)	0.36764(8)	1.0037(3)	0.0326(6)
C29	0.2939(3)	0.50960(8)	0.7483(3)	0.0375(7)

Table 2 (continued)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso} */ <i>U</i> _{eq}
C30	0.1494(4)	0.52558(9)	0.6386(3)	0.0545(9)
H30A	0.1574	0.5163	0.5511	0.082*
H30B	0.1454	0.5565	0.6408	0.082*
H30C	0.0550	0.5139	0.6553	0.082*
C31	0.4458(3)	0.52508(9)	0.7163(3)	0.0546(9)
H31A	0.5356	0.5129	0.7808	0.082*
H31B	0.4511	0.5560	0.7215	0.082*
H31C	0.4458	0.5160	0.6266	0.082*
C32	0.2854(4)	0.52938(8)	0.8830(3)	0.0512(9)
H32A	0.1914	0.5196	0.9048	0.077*
H32B	0.2832	0.5603	0.8756	0.077*
H32C	0.3764	0.5207	0.9533	0.077*
O5	0.1275(3)	0.45613(9)	1.1520(3)	0.0874(9)
H5A	0.2072	0.4409	1.1494	0.131*
H5B	0.1490	0.4656	1.2327	0.131*

Our research interest concerns the use of mixed ligands to give new molecular selfassembly architectures.

The X-ray single-crystal structural analysis reveals that the complex is a one-dimensional chain coordination polymer. The asymmetric unit of the title structure contains one Mn(II) ion, one *thip*^{2−} anion, one PYTPY ligand and one lattice water molecule. The Mn(II) center is five-coordinated *via* two oxygen atoms (Mn1–O1 = 2.093(2) Å and Mn1–O4#1 = 2.0876(19) Å, symmetry code: #1 *x*, *y*, *z* − 1) derived from two different *thip*^{2−} ligands and three nitrogen atoms (Mn1–N1 = 2.244(2) Å, Mn1–N2 = 2.202(2) Å, and Mn1–N3 = 2.249(2) Å) from one PYTPY ligand in a distorted tetragonal pyramidal coordination geometry, which are normal bond distances found in other Mn complexes [13, 14]. The completely deprotonated *thip*^{2−} ligand shows a monodentate coordination mode. Adjacent Mn(II) atoms are bridged by *thip*^{2−} ligands to form a single-chain structure, with the intra-chain Mn–Mn distance in the one-dimensional chain to be 10.229 Å. The coordinated PYTPY ligands are attached on one side of this chain. The neighboring one-dimensional chains are connected into two-dimensional structure *via* hydrogen bonding interactions among the uncoordinated carboxyl groups, lattice water molecules and uncoordinated pyridine nitrogen atoms.

Acknowledgements: This work was supported by the National Natural Science Foundation of China (No. 21671114).

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