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Crystal structure of poly[aqua- μ_2 -4,4'-bis(pyrid-4-yl)biphenyl- $\kappa^2 N:N'$]- μ_4 -4'-methyl-[1,1'-biphenyl]-3,5-dicarboxylato- $\kappa^4 O:O':O'':O'''$] manganese(II)], $C_{52}H_{40}N_2O_{10}Mn_2$

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.45 × 0.35 × 0.26 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.66 mm ⁻¹
Diffractometer, scan mode:	SuperNova, ω -scans
$\theta_{\max}$, completeness:	25.5°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	11721, 3974, 0.048
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2974
$N(\text{param})_{\text{refined}}$:	300
Programs:	CrysAlis ^{PRO} [1], SHELX [2], OLEX2 [3]

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

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Mn1	0.35544(4)	0.13369(4)	0.282625(9)	0.01968(14)
N1	0.4165(3)	0.1270(2)	0.33493(5)	0.0291(6)
O1	0.1123(2)	0.1707(2)	0.28738(5)	0.0402(6)
H1A	0.0545	0.1137	0.2793	0.060*
H1B	0.0874	0.2390	0.2787	0.060*
O2	0.1679(2)	0.40299(17)	0.26388(4)	0.0256(5)
O3	0.3716(2)	0.32517(18)	0.28970(4)	0.0298(5)
O4	0.0980(2)	0.88168(18)	0.27749(4)	0.0288(5)
O5	0.3342(2)	0.94278(17)	0.29192(4)	0.0282(5)
C1	0.3590(4)	0.2021(3)	0.35456(7)	0.0335(8)
H1	0.2813	0.2558	0.3481	0.040*
C2	0.4084(4)	0.2049(3)	0.38413(7)	0.0369(8)
H2	0.3636	0.2591	0.3969	0.044*
C3	0.5252(3)	0.1267(3)	0.39470(6)	0.0307(8)
C4	0.5842(4)	0.0488(3)	0.37411(7)	0.0347(8)
H4	0.6625	-0.0054	0.3799	0.042*
C5	0.5282(3)	0.0508(3)	0.34509(6)	0.0316(8)
H5	0.5699	-0.0034	0.3319	0.038*
C6	0.5873(4)	0.1273(3)	0.42589(7)	0.0365(8)
C7	0.5761(4)	0.2283(3)	0.44386(7)	0.0475(10)
H7	0.5257	0.2973	0.4365	0.057*
C8	0.6388(4)	0.2284(3)	0.47265(7)	0.0527(10)
H8	0.6290	0.2976	0.4842	0.063*
C9	0.7155(4)	0.1286(3)	0.48465(7)	0.0449(10)
C10	0.7261(5)	0.0276(3)	0.46666(8)	0.0582(11)
H10	0.7771	-0.0412	0.4740	0.070*
C11	0.6629(4)	0.0268(3)	0.43817(7)	0.0550(11)

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Abstract

$C_{52}H_{40}N_2O_{10}Mn_2$, monoclinic, $I2/a$ (no. 15), $a = 8.6162(4)$ Å, $b = 11.0217(5)$ Å, $c = 45.266(2)$ Å, $\beta = 92.828(4)^\circ$, $V = 4293.5(3)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0476$, $wR_{\text{ref}}(F^2) = 0.0988$, $T = 293(2)$ K.

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A part of the title crystal structure is shown in the figure ($B = 0.5 - x, 0.5 - y, 0.5 - z$; $C = 1.5 - x, y, 1 - z$; $D = x, -1 + y, z$). 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	0.6710	−0.0430	0.4268	0.066*
C12	0.3026(3)	0.5268(2)	0.29955(6)	0.0208(6)
C13	0.2393(3)	0.6347(3)	0.28854(6)	0.0200(6)
H13	0.1765	0.6345	0.2712	0.024*
C14	0.2700(3)	0.7427(2)	0.30347(6)	0.0196(6)
C15	0.3528(3)	0.7400(3)	0.33064(6)	0.0233(7)
H15	0.3726	0.8124	0.3407	0.028*
C16	0.4067(3)	0.6321(3)	0.34317(6)	0.0218(7)
C17	0.3865(3)	0.5267(3)	0.32662(6)	0.0233(7)
H17	0.4299	0.4546	0.3338	0.028*
C18	0.4817(3)	0.6297(3)	0.37360(6)	0.0254(7)
C19	0.4377(4)	0.7117(3)	0.39493(7)	0.0356(8)
H19	0.3648	0.7712	0.3898	0.043*
C20	0.5003(4)	0.7066(3)	0.42368(7)	0.0450(9)
H20	0.4679	0.7622	0.4375	0.054*
C21	0.6099(4)	0.6204(3)	0.43217(7)	0.0451(9)
C22	0.6555(4)	0.5401(3)	0.41094(7)	0.0434(9)
H22	0.7301	0.4818	0.4161	0.052*
C23	0.5931(3)	0.5441(3)	0.38215(7)	0.0358(8)
H23	0.6264	0.4885	0.3684	0.043*
C24	0.2795(3)	0.4101(3)	0.28281(6)	0.0210(6)
C25	0.2274(3)	0.8640(3)	0.28984(6)	0.0203(6)
C26	0.6765(5)	0.6131(4)	0.46368(8)	0.0840(16)
H26A	0.6062	0.5692	0.4755	0.126*
H26B	0.6909	0.6936	0.4715	0.126*
H26C	0.7748	0.5720	0.4640	0.126*

Source of material

A mixture of Mn(OAc)₂ · 4H₂O (0.024 g, 0.1 mmol), 4'-methyl-[1,1'-biphenyl]-3,5-dicarboxylic acid (0.1 mmol, 0.0256 g), 4, 4'-bis(pyrid-4-yl)biphenyl (0.1 mmol, 0.0308 g) and distilled water (10 mL) was heated in a 25 mL stainless steel reactor with a Teflon liner at 423 K for 30 h, followed by slow cooling to room temperature. Colourless crystals of the compound formed.

Experimental details

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

Discussion

The synthetic development of coordination polymers (CPs) continues to attract much attention because of their intriguing structural topologies and potential applications in gas storage, separation, sensing and heterogeneous catalysis [4–9]. The organic carboxylate ligands have been proven to be good candidates for the construction of CPs [10–12]. For example, polycarboxylates present versatile coordination modes to construct coordination polymers [13, 14].

Mixed multicarboxylate and nitrogen donor linkers have been widely utilized to construct CPs.

The asymmetric unit of the title structure contains one Mn(II) metal center, one 4'-methyl-[1,1'-biphenyl]-3,5-dicarboxylate ligand, and one 4,4'-bis(pyrid-4-yl)biphenyl ligand to construct a 3D-coordination polymer. The manganese atom is six-coordinated by one water ligand, by four oxygen atoms and one nitrogen atom. The Mn–O bond lengths range from 2.1211(18) to 2.1556(19) Å. The bond angles of O–Mn–O are in the range of 81.64(8)° to 173.65(8)°. All moieties are connected by hydrogen bonds $d(O(1) \cdots O(2)) = 2.822(3)$ Å, $d(O(1) \cdots O(4)A) = 3.218(3)$ Å, $d(O(1) \cdots O(5)B) = 2.719(3)$ Å. Symmetry codes: A $x, y - 1, z$; B $x - 1/2, -y + 1, z$.

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