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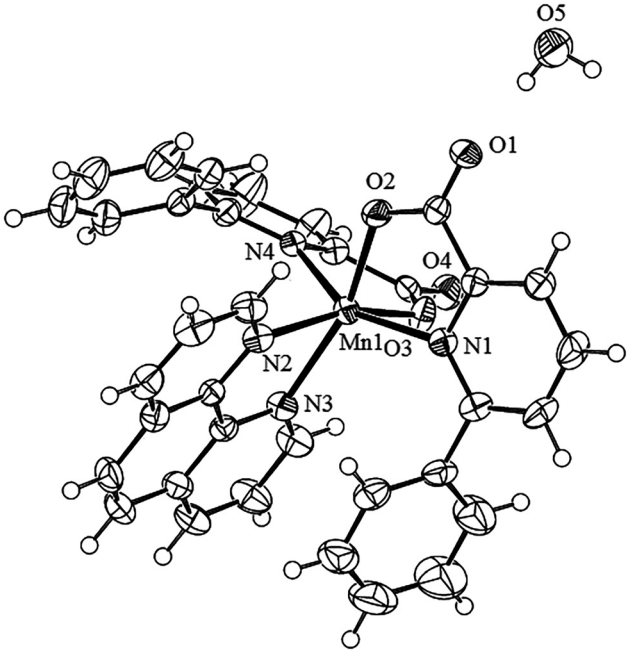
The crystal structure of [(1,10-phenantroline-κ²*N*,*N*′)-bis(6-phenylpyridine-2-carboxylato-κ²*N*,*O*)manganese(II)] monohydrate, $C_{36}H_{26}N_4O_5Mn$



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Abstract

$C_{36}H_{26}N_4O_5Mn$, orthorhombic, $P2_12_12_1$ (no. 19), a = 10.7134(7) Å, b = 10.7573(10) Å, c = 26.6304(18) Å, β = 90°, V = 3069.1(4) Å^3, Z = 4, $R_{gt}(F)$ = 0.0454, $wR_{ref}(F^2)$ = 0.0890, T = 220 K.

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The molecular structure is shown in the Figure. 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:	Yellow block
Size:	0.14 × 0.12 × 0.10 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.48 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	29.6°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	10781, 6672, 0.028
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 5530
$N(param)_{refined}$:	418
Programs:	Bruker [1], Olex2 [2], SHELX [3], CrysAlis^{PRO} [4]

Source of material

The title complex was synthesized according to literature [5] method. Ten milliliter aqueous solution of 0.5 mmol ligand (6-phenylpyridine-2-carboxylic acid, 199.2 mg) and 0.5 mmol NaOH (20 mg) was added to 15 mL ethanol solution of 0.25 mmol $Mn(O_2CMe)_2{\cdot}4H_2O$ (0.0612 mg) with molar ratio 2:1 (L:M). Then 5 mL of an ethanol solution of 0.25 mmol 1,10-phenanthroline monohydrate (45 mg) was added. The mixture was stirred at 75 °C for 4 h, cooled to room temperature, and continued to stir for 3 h, then filtered. After the filtrate was resting for 16 days, yellow crystals of the title complex were obtained in yield 68%. **Anal. Calcd.** for $C_{36}H_{26}N_4O_5Mn$: C, 66.51; H, 4.00; N, 8.62. Found: C, 66.76; H, 4.39; N, 8.37.

Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.93 Å and O–H = 0.85 Å). Their U_{iso} values were set to 1.2U_{eq} or 1.5U_{eq} of the parent atoms. The Flack parameter (0.006(12)) was determined using 1814 quotients [2].

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.30189 (4)	0.82269 (5)	0.65684 (2)	0.02649 (13)
O1	0.2121 (2)	0.8576 (2)	0.80707 (8)	0.0358 (6)
O2	0.3116 (2)	0.8189 (2)	0.73585 (8)	0.0364 (6)
O3	0.1462 (2)	0.7091 (2)	0.64264 (10)	0.0362 (6)
O4	0.0740 (2)	0.5211 (3)	0.62318 (10)	0.0395 (7)
N1	0.1599 (2)	0.9706 (3)	0.68408 (10)	0.0270 (7)
N2	0.4631 (2)	0.9553 (3)	0.64808 (10)	0.0284 (6)
N3	0.3503 (3)	0.8301 (3)	0.57309 (10)	0.0294 (6)
N4	0.3820 (2)	0.6182 (3)	0.65208 (11)	0.0258 (6)
C1	0.1049 (4)	1.0566 (3)	0.60280 (14)	0.0348 (9)
C2	0.2145 (4)	1.1038 (3)	0.58413 (16)	0.0419 (10)
H2	0.276840	1.128244	0.606341	0.050*
C3	0.5257 (3)	0.4503 (4)	0.63966 (17)	0.0490 (12)
H3	0.607187	0.420608	0.641024	0.059*
C4	0.1427 (5)	1.0803 (5)	0.50008 (19)	0.0694 (15)
H4	0.155280	1.087444	0.465652	0.083*
C5	0.0319 (6)	1.0340 (6)	0.51815 (19)	0.0870 (19)
H5	−0.030485	1.010132	0.495845	0.104*
C6	0.0124 (5)	1.0224 (5)	0.56969 (17)	0.0647 (14)
H6	−0.063026	0.991670	0.581708	0.078*
C7	0.0840 (3)	1.0469 (3)	0.65809 (14)	0.0310 (8)
C8	−0.0098 (4)	1.1144 (4)	0.68097 (16)	0.0402 (10)
H8	−0.060713	1.166650	0.662132	0.048*
C9	−0.0271 (4)	1.1033 (4)	0.73234 (16)	0.0444 (10)
H9	−0.089470	1.148257	0.748493	0.053*
C10	0.0495 (3)	1.0247 (3)	0.75909 (13)	0.0334 (9)
H10	0.039071	1.014665	0.793525	0.040*
C11	0.1419 (3)	0.9612 (3)	0.73386 (13)	0.0270 (8)
C12	0.2278 (3)	0.8726 (3)	0.76188 (13)	0.0263 (8)
C13	0.1581 (3)	0.5939 (3)	0.63443 (12)	0.0280 (8)
C14	0.2904 (3)	0.5408 (3)	0.63719 (12)	0.0290 (8)
C15	0.3102 (4)	0.4191 (4)	0.62305 (16)	0.0451 (10)
H15	0.244343	0.368666	0.612915	0.054*
C16	0.4307 (4)	0.3744 (4)	0.6244 (2)	0.0610 (14)
H16	0.447353	0.292831	0.614968	0.073*
C17	0.2344 (5)	1.1161 (4)	0.53282 (18)	0.0555 (13)
H17	0.309313	1.148146	0.520834	0.067*
C18	0.4994 (3)	0.5726 (3)	0.65314 (14)	0.0295 (8)
C19	0.6023 (3)	0.6560 (3)	0.67063 (13)	0.0301 (8)
C20	0.7157 (3)	0.6574 (4)	0.64465 (14)	0.0404 (9)
H20	0.725321	0.608529	0.616106	0.048*
C21	0.8123 (3)	0.7298 (4)	0.66076 (18)	0.0513 (11)
H21	0.886654	0.731561	0.642727	0.062*
C22	0.8001 (4)	0.8005 (4)	0.70372 (17)	0.0511 (11)
H22	0.866154	0.849428	0.714766	0.061*
C23	0.6894 (4)	0.7983 (4)	0.73027 (16)	0.0484 (10)
H23	0.681330	0.844853	0.759518	0.058*
C24	0.5907 (3)	0.7270 (3)	0.71337 (14)	0.0356 (9)
H24	0.515857	0.727031	0.731027	0.043*
C25	0.2934 (4)	0.7708 (3)	0.53626 (13)	0.0393 (9)
H25	0.223646	0.723204	0.544077	0.047*
C26	0.3319 (4)	0.7755 (4)	0.48631 (14)	0.0461 (11)
H26	0.290085	0.729981	0.461837	0.055*
C27	0.4322 (4)	0.8482 (4)	0.47378 (14)	0.0401 (10)
H27	0.458916	0.853085	0.440611	0.048*
C28	0.4943 (3)	0.9150 (3)	0.51146 (13)	0.0314 (8)
C29	0.4506 (3)	0.9017 (3)	0.56105 (13)	0.0258 (7)
C30	0.5093 (3)	0.9703 (3)	0.60086 (13)	0.0254 (7)
C31	0.6088 (3)	1.0511 (3)	0.59010 (15)	0.0310 (8)
C32	0.6504 (3)	1.0625 (4)	0.53906 (16)	0.0403 (10)
H32	0.716232	1.115766	0.531593	0.048*
C33	0.5959 (3)	0.9975 (4)	0.50173 (15)	0.0386 (10)
H33	0.624942	1.006544	0.469032	0.046*
C34	0.6598 (3)	1.1191 (3)	0.62982 (15)	0.0374 (9)
H34	0.725877	1.173359	0.624115	0.045*
C35	0.6123 (4)	1.1055 (4)	0.67693 (16)	0.0414 (10)
H35	0.644718	1.150974	0.703624	0.050*
C36	0.5135 (3)	1.0217 (4)	0.68455 (14)	0.0372 (9)
H36	0.482033	1.012570	0.716885	0.045*
O5	0.1350 (3)	0.8637 (3)	0.90596 (11)	0.0610 (9)
H5A	0.067930	0.905822	0.906289	0.092*
H5B	0.159817	0.867308	0.875659	0.092*

Comment

The preparation and characterization of metal complexes is part of our active area of research [6]. For example, metal complexes can generate 1D, 2D, or 3D supermolecular structures [7], and show potential applications such as anticancer agents [8], antibacterial activities [9], molecular magnets [10], catalytic activities [11]. According to the investigations of our research group, 6-phenylpyridine-2-carboxylate is an excellent bidentate ligand, up to now, its Co(II), Cu(II), Zn(II) and Pb(II) complexes have been synthesized and structural characterized [5, 12–15].

In this paper, we have also synthesized an characterized another metal complex, (1,10-phenantroline-κ^2N,N')-bis(6-phenylpyridine-2- carboxylato-κ^2N,O)manganese(II)]monohydrate **(1)** using 6-phenylpyridine-2-carboxylic acid, $Mn(O_2CMe)_2{\cdot}4H_2O$, 1,10- phenantroline and NaOH as the raw material. The structural analysis of **1** indicates that it crystallizes in the space group $P2_12_12_1$. The molecular structure of **1** is shown in the Figure. **1** is composed of a Mn(II) ion, two bidentate 6-phenylpyridine-2-carboxylate ligands, one 1,10-phenantroline ligand, and one lattice water molecule. The Mn(II) is six-coordinated by two 6-phenylpyridine-2-carboxylate ligands connected to Mn(II) in a bidentate coordinating fashion by two pyridine nitrogen atoms (N1 and N4) and two oxygen atoms (O2 and O3) of carboxylate groups, as well as two nitrogen atoms (N2 and N3) of one 1,10-phenantroline ligand. The coordination geometry of Mn(II) is distorted octahedral. The bond angle of O2–Mn1–N3 is 164.07(10)° and the summation of bond angles (N1–Mn1–N2,95.78(10)°, N4–Mn1–N2,107.79(10)°,

N4–Mn1–O3, 74.77(9)° and N1–Mn1–O3,86.26(9)°) is 364.6°, showing that MnN1N2N4O3 located on the equatorial plane and O2N3 are in the axial position. The hydrogen bonds (O5–H5A···O4 and O5–H5A···O1) between the water molecules and oxygen atoms of the 6-phenylpyridine-2-carboxylate ligands play an important role in the formation of 3D network structure of the complexes.

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

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