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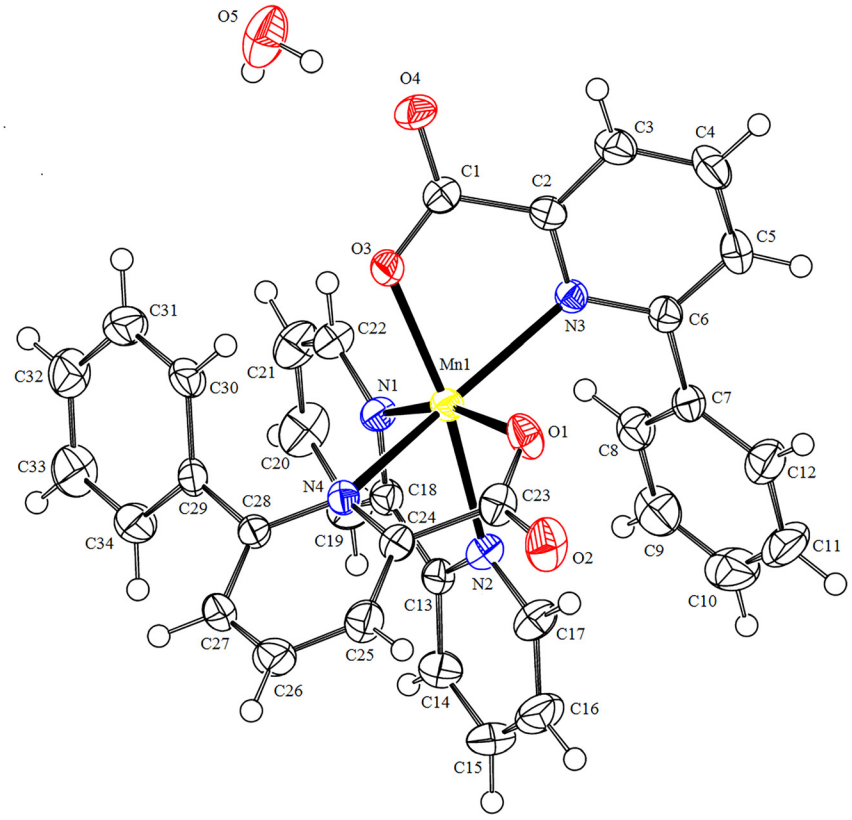
The crystal structure of (2,2′-bipyridine-κ²*N*,*N*′)-bis(6-phenylpyridine-2-carboxylate-κ²*N*,*O*) manganese(II)] monohydrate, $C_{34}H_{26}N_4O_5Mn$



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Abstract

$C_{34}H_{26}N_4O_5Mn$, monoclinic, *C2/c* (no. 15), $a = 29.4330(18)$ Å, $b = 10.4120(6)$ Å, $c = 20.0207(12)$ Å, $\beta = 107.246(6)°$, $V = 5859.6(6)$ Å^3, $Z = 8$, $R_{gt}(F) = 0.0380$, $wR_{ref}(F^2) = 0.0865$, T = 200 K.

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Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.13 × 0.11 × 0.10 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.50 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	25.0°, 99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	12,338, 5098, 0.031
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 4194
$N(param)_{refined}$:	400
Programs:	Bruker [1], Olex2 [2], SHELX [3], CrysAlis^{PRO} [4]

The molecular structure is shown in figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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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	0.37807 (2)	0.43142 (3)	0.30545 (2)	0.02237 (11)
O1	0.38599 (5)	0.50595 (16)	0.40672 (7)	0.0334 (4)
O2	0.35953 (5)	0.49287 (18)	0.50022 (7)	0.0430 (4)
O3	0.36618 (5)	0.59596 (15)	0.24053 (8)	0.0314 (4)
O4	0.39641 (5)	0.77791 (15)	0.21317 (8)	0.0336 (4)
N1	0.37197 (6)	0.29853 (17)	0.21492 (8)	0.0251 (4)
N2	0.38528 (6)	0.22550 (18)	0.34772 (9)	0.0262 (4)
N3	0.45280 (5)	0.52288 (17)	0.32239 (8)	0.0220 (4)
N4	0.30241 (6)	0.41577 (16)	0.32208 (8)	0.0215 (4)
C1	0.39946 (7)	0.6769 (2)	0.24683 (10)	0.0253 (5)
C2	0.44662 (7)	0.6454 (2)	0.30033 (10)	0.0243 (5)
C3	0.48084 (8)	0.7391 (2)	0.32451 (12)	0.0325 (5)
H3	0.475718	0.822610	0.307502	0.039*
C4	0.52276 (8)	0.7062 (2)	0.37439 (12)	0.0381 (6)
H4	0.545919	0.768056	0.392630	0.046*
C5	0.52983 (8)	0.5810 (2)	0.39674 (12)	0.0333 (6)
H5	0.557993	0.557168	0.430013	0.040*
C6	0.49473 (7)	0.4905 (2)	0.36937 (10)	0.0248 (5)
C7	0.50193 (7)	0.3533 (2)	0.38936 (11)	0.0276 (5)
C8	0.48914 (8)	0.2586 (2)	0.33824 (12)	0.0337 (6)
H8	0.475584	0.281799	0.291707	0.040*
C9	0.49642 (9)	0.1301 (3)	0.35600 (15)	0.0462 (7)
H9	0.488297	0.067377	0.321406	0.055*
C10	0.51578 (9)	0.0952 (3)	0.42528 (17)	0.0545 (8)
H10	0.520107	0.008912	0.437489	0.065*
C11	0.52868 (9)	0.1887 (3)	0.47630 (15)	0.0516 (7)
H11	0.541602	0.164937	0.522864	0.062*
C12	0.52259 (8)	0.3171 (3)	0.45888 (12)	0.0394 (6)
H12	0.532254	0.379437	0.493458	0.047*
C13	0.37552 (7)	0.1310 (2)	0.29929 (10)	0.0259 (5)
C14	0.36972 (8)	0.0049 (2)	0.31701 (13)	0.0391 (6)
H14	0.363330	−0.059004	0.283042	0.047*
C15	0.37350 (9)	−0.0251 (3)	0.38575 (13)	0.0467 (7)
H15	0.368877	−0.108934	0.398367	0.056*
C16	0.38415 (9)	0.0702 (3)	0.43487 (13)	0.0449 (7)
H16	0.387340	0.052048	0.481513	0.054*
C17	0.39004 (8)	0.1932 (2)	0.41427 (11)	0.0340 (6)
H17	0.397723	0.257301	0.448127	0.041*
C18	0.37255 (7)	0.1708 (2)	0.22656 (10)	0.0249 (5)
C19	0.37129 (8)	0.0829 (2)	0.17441 (12)	0.0379 (6)
H19	0.371897	−0.004749	0.183533	0.045*
C20	0.36910 (9)	0.1271 (3)	0.10853 (12)	0.0447 (7)
H20	0.367814	0.069118	0.072657	0.054*
C21	0.36884 (9)	0.2566 (3)	0.09614 (12)	0.0408 (6)
H21	0.367896	0.287914	0.052247	0.049*
C22	0.37002 (7)	0.3393 (2)	0.15052 (10)	0.0310 (5)
H22	0.369428	0.427189	0.142162	0.037*
C23	0.35482 (8)	0.4804 (2)	0.43699 (11)	0.0291 (5)
C24	0.30783 (7)	0.4261 (2)	0.39139 (10)	0.0244 (5)
C25	0.27337 (8)	0.3874 (2)	0.42120 (11)	0.0335 (6)
H25	0.277907	0.397960	0.468863	0.040*
C26	0.23224 (8)	0.3328 (3)	0.37925 (12)	0.0380 (6)
H26	0.208790	0.304268	0.398257	0.046*
C27	0.22632 (7)	0.3211 (2)	0.30880 (12)	0.0330 (6)
H27	0.198808	0.283708	0.279840	0.040*
C28	0.26136 (7)	0.3651 (2)	0.28072 (10)	0.0244 (5)
C29	0.25381 (7)	0.3635 (2)	0.20402 (10)	0.0255 (5)
C30	0.26418 (8)	0.4722 (2)	0.17105 (11)	0.0316 (5)
H30	0.277834	0.543242	0.197668	0.038*
C31	0.25442 (8)	0.4762 (3)	0.09889 (12)	0.0405 (6)
H31	0.261174	0.549901	0.077342	0.049*
C32	0.23470 (9)	0.3708 (3)	0.05920 (12)	0.0429 (6)
H32	0.228332	0.372987	0.010853	0.051*
C33	0.22454 (9)	0.2632 (3)	0.09106 (13)	0.0465 (7)
H33	0.211272	0.192088	0.064192	0.056*
C34	0.23381 (8)	0.2589 (2)	0.16303 (12)	0.0394 (6)
H34	0.226542	0.185130	0.184017	0.047*
O5	0.36059 (7)	0.7588 (2)	0.06569 (9)	0.0549 (5)
H5A	0.358793	0.681576	0.051234	0.082*
H5B	0.371939	0.759905	0.110035	0.082*

Source of material

The title compound was synthesized similar to that reported in the literature [5]. In 15 mL distilled H_2O, 199.2 mg 6-phenylpyridine-2-carboxylic acid (1.0 mmol), 122.5 mg $Mn(O_2CMe)_2{\cdot}4H_2O$ (0.5 mmol) and 40 mg NaOH (1.0 mmol) were dissolved with stirring. Then 78 mg 2,2′-bipyridine (0.5 mmol) and 15 mL ethanol were added to the above solution and the resulting mixture was gradually heated up to 75 °C and remained at this temperature for further reaction for 6 h. After the reaction was stopped and cooled naturally to room temperature, it was filtered. The yellow crystals of the title compound were obtained in one weeks. **Anal. Calcd.** for $C_{34}H_{26}N_4O_5Mn$: C, 65.22; H, 4.16; N, 8.95. Found: C, 64.96; H, 4.49; N, 8.67.

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.

Comment

Studies on the synthesis, structural characterization and property of Mn(II) complexes have attracted great interest during the past decades [6]. They exhibited structural diversities and a wide range of potential applications including electrocatalytic properties [7], antioxidant activity [8], electrochemical oxygen reduction reaction [9], fluorescence studies and cytotoxicity [10]. As an excellent

multidentate ligand, 6-phenylpyridine-2-carboxylic acid has a strong affinity for many metal ions. Up to now, our group reported its Co(II), Cu(II), Zn(II) and Pb(II) complexes and determined their crystal structures [11–15]. To continue to investigate its coordination behavior with other metal ions, a new Mn(II) complex has been synthesized and structural characterized. The Mn(II) complex consists of a Mn(II) ion, two 6-phenylpyridine-2-carboxylate ligands, one 2,2′-bipyridine ligand, and one lattice water molecule. The molecular structure is shown in figure, it shows that the coordination mode of 2,2′-bipyridine and 6-phenylpyridine-2-carboxylate ligands is the same as reported for other complexes [5, 14, 15]. In the title structure both two 6-phenylpyridine-2-carboxylate ligands and one 2,2′-bipyridine ligand are coordinated to Mn(II) with a bidentate chelating fashion by four pyridine nitrogens and two oxygens of carboxylate groups. The Mn(II) is six-coordinated with two nitrogen atoms (N3 and N4), two oxygen atoms (O1 and O3) from two 6-phenylpyridine-2-carboxylate ligands, and two nitrogen atoms (N1 and N2) from one 2,2′-bipyridine ligand, giving a distorted octahedral coordination geometry. The bond angle of O3–Mn1–N2 is 164.73(6)° and the sum of bond angles N1–Mn1–N4 (102.66(6)°), N4–Mn1–O1 (74.34(5)°), N3–Mn1–O1 (83.09(6)°) and N1–Mn1–N3 (102.46(6)°) equals 362.55° indicates the Mn1 is on the center of the N1–N4–O1–N3 plane. All the Mn–O and Mn–N distances are 2.1182(14) Å (Mn1–O1), 2.1160(15) Å (Mn1–O3), 2.2448(17) Å (Mn1–N1), 2.2916(18) Å (Mn1–N2), 2.3276(16) Å (Mn1–N3), 2.3530(16) Å (Mn1–N4), respectively. The intermolecular hydrogen-bonding (O–H···O) interactions allow the complex molecule to form a one-dimensional chain structure.

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

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