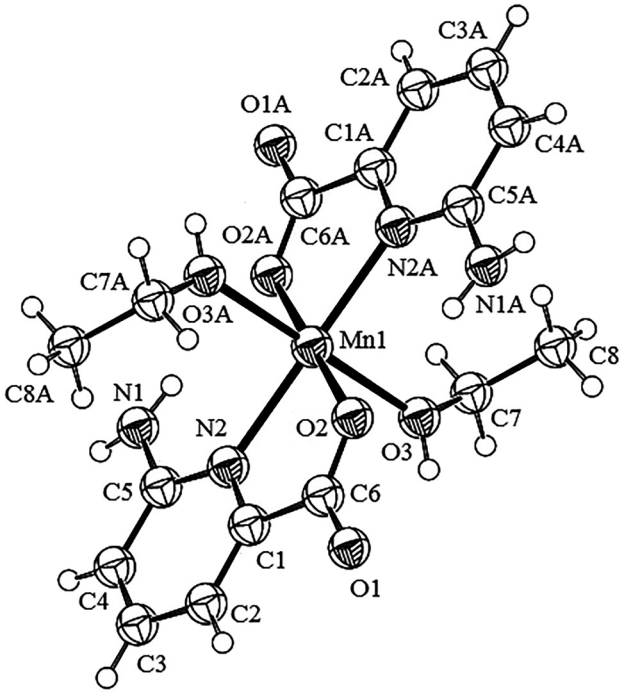
Tai Xi-Shi*, Zhang Li-Li, Liu Li-Li, Cao Shu-Hua and Wang Li-Hua

The crystal structure of bis(ethanol-k*O*)-bis(6-aminopicolinato-k^2*N*,*O*)manganese(II), $C_{16}H_{22}O_6N_4Mn$



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Abstract

$C_{16}H_{22}O_6N_4Mn$, triclinic, $P\bar{1}$ (no. 2), a = 7.4412(6) Å, b = 8.2273(7) Å, c = 8.6693(7) Å, α = 72.516(7)°, β = 76.827(7)°, γ = 63.444(9)°, V = 450.08(7) Å^3, Z = 1, $R_{gt}(F)$ = 0.0378, $wR_{ref}(F^2)$ = 0.0755, T = 150(1) K.

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The molecular structure is shown in the figure (All atoms are drawn with an arbitrary radius; A = –x, 1–y, 1–z).

***Corresponding author: Tai Xi-Shi,** College of Chemistry and Chemical Engineering, Weifang University, Weifang, Shandong 261061, P.R. China, E-mail: taixs@wfu.edu.cn. https://orcid.org/0000-0002-0050-1900

Zhang Li-Li, Liu Li-Li, Cao Shu-Hua and Wang Li-Hua, College of Chemistry and Chemical Engineering, Weifang University, Weifang, Shandong 261061, P.R. China

Table 1: Data collection and handling.

Crystal:	Colourless block
Size:	0.11 × 0.10 × 0.08 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	0.78 mm^{-1}
Diffractometer, scan mode:	SuperNova, ω
θ_{max}, completeness:	25.0°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	2860, 1575, 0.040
Criterion for I_{obs}, $N(hkl)_{gt}$:	I_{obs} > 2 σ(I_{obs}), 1379
$N(param)_{refined}$:	131
Programs:	Bruker [1], Olex2 [2], SHELX [3], Diamond [4]

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

Source of material

0.1381 g 2–Amino-6-pyridinecarboxylic acid (1.0 mmol) and 0.0675 g 2,5-pyridinedicarbaldehyde (0.5 mmol) were dissolved in a 10 mL water-ethanol solution (v:v = 1:1) at room temperature. After 10 min, 0.1225 g manganese acetate tetrahydrate (0.5 mmol) solid was added to the aforementioned solution. The mixture was stirred for 4 h at 75 °C and cooled to room temperature. The colorless crystals of the title compound were received from the filtrate in 20 days.

Experimental details

The hydrogen atoms were positioned geometrically (C–H = 0.93–0.97 Å, O–H = 0.82 Å and N–H = 0.83–0.86 Å). Their U_{iso} values were set to 1.2U_{eq} or 1.5U_{eq} of the parent atoms.

Comment

Many pyridine derivatives containing metal complexes exhibit abundant coordination structures and properties in

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Mn1	0.000000	0.500000	0.500000	0.01335 (17)
O1	0.4112 (2)	0.5829 (2)	0.6870 (2)	0.0178 (4)
O2	0.1380 (2)	0.6283 (2)	0.5891 (2)	0.0161 (4)
O3	0.2053 (2)	0.5222 (2)	0.27178 (19)	0.0200 (4)
H3	0.321480	0.503876	0.278002	0.030*
N1	0.1744 (3)	0.0240 (3)	0.6054 (3)	0.0210 (5)
H1A	0.228888	−0.095224	0.617652	0.025*
H1B	0.090 (4)	0.102 (3)	0.543 (3)	0.022 (8)*
N2	0.2513 (3)	0.2605 (2)	0.6251 (2)	0.0128 (4)
C1	0.3690 (3)	0.3147 (3)	0.6799 (3)	0.0127 (5)
C2	0.5334 (4)	0.1900 (3)	0.7598 (3)	0.0204 (6)
H2	0.612269	0.230854	0.794440	0.024*
C3	0.5802 (4)	−0.0002 (3)	0.7883 (3)	0.0261 (6)
H3A	0.691190	−0.088004	0.842659	0.031*
C4	0.4631 (4)	−0.0562 (3)	0.7364 (3)	0.0215 (6)
H4	0.493142	−0.182559	0.755187	0.026*
C5	0.2963 (3)	0.0772 (3)	0.6542 (3)	0.0145 (5)
C6	0.3035 (3)	0.5244 (3)	0.6486 (3)	0.0126 (5)
C7	0.1831 (4)	0.5395 (3)	0.1066 (3)	0.0244 (6)
H7A	0.098184	0.477993	0.106609	0.029*
H7B	0.314730	0.476136	0.051266	0.029*
C8	0.0925 (4)	0.7376 (3)	0.0150 (3)	0.0285 (7)
H8A	0.074476	0.741410	−0.092428	0.043*
H8B	0.180917	0.796806	0.007466	0.043*
H8C	−0.036081	0.802186	0.070867	0.043*

luminescence, biological activity, catalysis and magnetics [5, 6]. Therefore, more and more attention has been paid to the study of substituted pyridine based metal complexes. Our group has also done research in this area [7, 8]. In our previous work, two new Mg(II) complexes, bis(ethanol-k*O*)-bis(6-aminopicolinato-k^2*N*,*O*)magnesium(II) and diaqua-bis(6-aminopicolinato-k^2*N*,*O*)magnesium(II), have been reported [9, 10]. In this work, we determined the structure of a new Mn(II) complex.

The Mn(II) title complex contains one Mn(II) ion, two 2-amino-6-pyridinecarboxylate ligands and two coordinanted ethanol molecules. The Mn(II) ion is coordinated with four O atoms (O2, O2A, O3 and O3A) and two N atoms (N2 and N2A) from two different 2-amino-6-pyridinecarboxylate ligands and two different coordinated ethanol molecules, which forms a six-coordinated distorted octahedral coordination environment. The bond lengths are 2.1411(15) Å (Mn–O2 and Mn–O2A), 2.2220(15) Å (Mn–O3 and Mn–O3A) and 2.2142(19) Å (Mn–N2 and Mn–N2A), respectively. These geometric parameters are consistent with those reported in the literature [9, 10]. The intramolecular hydrogen bonds (NH···O) play an important role in the formation of Mn(II) complex structure. The Mn(II) complexes form a one-dimensional chain structure due to the intermolecular OH···O hydrogen bonds.

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

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