Crystal structure of catena-(2,2'-bipyridyl-$\kappa^2 N,N$)-μ_2(pyridine-2,3-dicarboxylato-$\kappa^3 N,O:O'$)manganese(II)monohydrate, $[Mn(C_7H_3NO_4)(C_{10}H_8N_2)(H_2O)]_n \cdot nH_2O$, $C_{17}H_{15}MnN_3O_6$

Chuang Zhang, Ling-Yu Zhang, Shu-Long Wang and Qin Huang*

College of Chemistry and Chemical Engineering, Guangxi University for Nationalities, Nanning 530006, Guangxi Province, P. R.China

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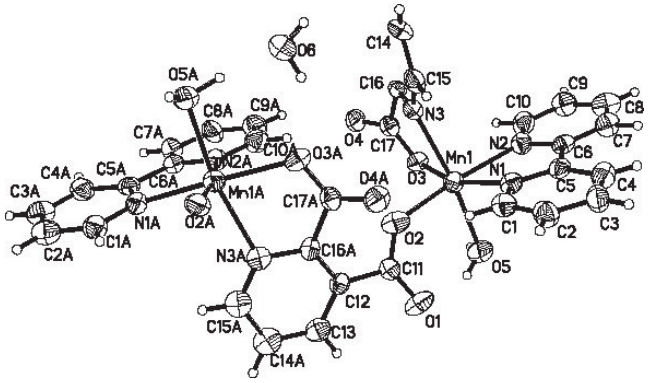

Abstract

$C_{17}H_{15}MnN_3O_6$, monoclinic, $P2_1/c$ (no. 14), a = 11.136(3) Å, b = 10.809(3) Å, c = 14.111(4) Å, β = 92.059(4)°, V = 1697.4 Å^3, Z = 4, $R_{gt}(F)$ = 0.0402, $wR_{ref}(F^2)$ = 0.0564, T = 296 K.

Table 1. Data collection and handling.

Crystal:	yellow blocks, size 0.18×0.25×0.28 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	8.20 cm^{-1}
Diffractometer, scan mode:	CCD area detector, φ and ω
$2\theta_{max}$:	54.96°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	10834, 3853
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2138
$N(param)_{refined}$:	244
Programs:	SHELX [2]

Source of material

A 5 mL aqueous solution of $MnCl_2 \cdot 4H_2O$ (99 mg, 0.5 mmol) was added to 5 mL of an aqueous solution of pyridine-2,3-dicarboxylic acid (*pydc*, 83.5 mg, 0.5 mmol) and 2,2'-bipyridine (*bipy*, 78 mg, 0.5 mmol). The mixture was strirred for fifteen hours, then was placed in a Parr Teflon-lined stainless steel vessel (25cm^3), and heated at 403 K for 3 days. After slow cooling to room temperature, yellow block shaped crystals were obtained.

Discussion

Because of the diversity of the coordination modes and high structural stability, pyridine-dicarboxylic acid ligands has drawn a wide attention [1]. To better understand the coordination chemistry of 2,3-*pydc* and prepare novel materials, we synthesized the title polymeric complex. In the title complex structure, the distorted octahedron is formed by sixfold coordinated Mn metal center and three nitrogen atoms and 4 oxygen atoms from the ligands. Here, the Mn(II) ion is axialy bonded to one O atom from the water molecules (d(Mn1–O5) = 2.222(2) Å) and one N atom from the *pydc* ligand (d(Mn1–N3) = 2.276(2) Å). The equatorial sites are occupied by two O atom from two different *pydc* ligands (d(Mn1–O2) = 2.0858(5) Å, d(Mn1–O3) = 2.169(2) Å) and two N atom belonging to one *bipy* (d(Mn1–N1) = 2.249(2) Å, d(Mn1–N2) = 2.262(2) Å). The bond distance are similar to those be reported in other octahedral Mn(II) complexes. The Mn(II) ions are bridged by *pydc* ligand to form the 1D polymeric chain along [010]. In the complex, intermolecular O–H···O hydrogen bonds play an important role. The coordinated water molecule (O5) is connected to the oxygen atom O1 of one carboxy group. The other water molecule interlinks the adjoining polymeric chains by strong hydrogen bonds to a 2D network. The relevant distances are d(O6–H10···O3^{i}) = 2.829(2) Å, d(O5–H8···O6^{ii}) = 2.736(2) Å, d(O6–H9···O4^{iii}) = 2.752(3) Å, d(O5–H5···O1) = 2.737(2) Å. (symmetry codes **i**: $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; **ii**: $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; **iii**: $x, -y+\frac{1}{2}, z+\frac{1}{2}$).

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(5C)	4*e*	0.2100	0.1115	0.0647	0.052
H(5A)	4*e*	0.1794	0.2344	0.0683	0.052
H(15)	4*e*	0.1777	0.4240	0.3134	0.047
H(23)	4*e*	0.0056	0.4830	0.3860	0.054
H(24)	4*e*	–0.1257	0.3332	0.4370	0.055
H(20)	4*e*	–0.0794	0.1260	0.4136	0.051
H(19)	4*e*	–0.0169	–0.0608	0.4042	0.050
H(21)	4*e*	0.0526	–0.2587	0.3783	0.056
H(22)	4*e*	0.2270	–0.2879	0.2968	0.054
H(18)	4*e*	0.3261	–0.1171	0.2424	0.050
H(13)	4*e*	0.3268	0.5798	–0.0249	0.047
H(7)	4*e*	0.5433	0.2433	0.5518	0.053
H(6)	4*e*	0.4016	0.2942	0.4356	0.049
H(6C)	4*e*	0.6467	0.5099	0.4517	0.065
H(6D)	4*e*	0.6676	0.4809	0.5462	0.065

* Correspondence author (e-mail: chuang0203@126.com)

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Mn(1)	4*e*	0.30280(3)	0.18077(3)	0.22775(3)	0.0316(2)	0.0325(2)	0.0340(3)	0.0010(2)	0.0011(2)	0.0018(2)
N(1)	4*e*	0.1536(2)	0.2443(2)	0.3194(1)	0.032(1)	0.033(1)	0.036(2)	–0.002(1)	–0.002(1)	0.000(1)
N(2)	4*e*	0.2168(2)	0.0102(2)	0.2887(1)	0.034(1)	0.035(1)	0.033(2)	0.002(1)	0.002(1)	0.002(1)
N(3)	4*e*	0.4576(2)	0.1823(2)	0.3376(2)	0.036(1)	0.034(1)	0.031(1)	0.004(1)	0.003(1)	–0.005(1)
O(1)	4*e*	0.2208(1)	0.4141(2)	0.0703(1)	0.038(1)	0.049(1)	0.062(2)	–0.0104(9)	–0.020(1)	0.010(1)
O(2)	4*e*	0.3578(1)	0.3533(1)	0.1792(1)	0.049(1)	0.036(1)	0.040(1)	–0.0075(9)	–0.0100(9)	0.010(1)
O(3)	4*e*	0.4397(1)	0.0646(1)	0.1679(1)	0.033(1)	0.047(1)	0.036(1)	0.0033(9)	–0.0066(9)	–0.005(1)
O(4)	4*e*	0.6393(1)	0.0426(2)	0.1788(1)	0.036(1)	0.058(1)	0.034(1)	0.0044(9)	0.0068(9)	–0.004(1)
O(5)	4*e*	0.1813(1)	0.1674(1)	0.0998(1)	0.049(1)	0.042(1)	0.039(1)	–0.0023(9)	–0.0060(9)	0.001(1)
C(1)	4*e*	0.1254(2)	0.3632(2)	0.3338(2)	0.041(2)	0.038(2)	0.039(2)	–0.001(1)	–0.002(2)	–0.000(2)
C(2)	4*e*	0.0222(2)	0.3996(3)	0.3774(2)	0.050(2)	0.042(2)	0.044(2)	0.011(2)	–0.001(2)	–0.004(2)
C(3)	4*e*	–0.0554(2)	0.3109(3)	0.4077(2)	0.039(2)	0.061(2)	0.038(2)	0.013(2)	0.004(1)	–0.002(2)
C(4)	4*e*	–0.0276(2)	0.1877(3)	0.3940(2)	0.038(2)	0.053(2)	0.037(2)	0.001(2)	0.004(1)	0.007(2)
C(5)	4*e*	0.0780(2)	0.1568(2)	0.3510(2)	0.030(1)	0.039(2)	0.026(2)	0.002(1)	–0.004(1)	0.003(1)
C(6)	4*e*	0.1159(2)	0.0266(2)	0.3367(2)	0.032(2)	0.038(2)	0.029(2)	–0.003(1)	–0.006(1)	0.003(1)
C(7)	4*e*	0.0528(2)	–0.0733(2)	0.3711(2)	0.042(2)	0.043(2)	0.042(2)	–0.007(1)	0.003(2)	0.006(2)
C(8)	4*e*	0.0945(2)	–0.1910(2)	0.3558(2)	0.056(2)	0.037(2)	0.047(2)	–0.014(2)	–0.005(2)	0.011(2)
C(9)	4*e*	0.1975(2)	–0.2087(2)	0.3075(2)	0.053(2)	0.031(2)	0.051(2)	0.001(1)	–0.003(2)	0.002(2)
C(10)	4*e*	0.2559(2)	–0.1059(2)	0.2752(2)	0.039(2)	0.038(2)	0.050(2)	0.006(1)	–0.002(2)	0.001(2)
C(11)	4*e*	0.3122(2)	0.4305(2)	0.1214(2)	0.034(2)	0.038(2)	0.032(2)	0.001(1)	0.004(1)	–0.003(1)
C(12)	4*e*	0.3827(2)	0.5490(2)	0.1103(2)	0.029(1)	0.028(1)	0.029(2)	0.003(1)	–0.001(1)	0.005(1)
C(13)	4*e*	0.3808(2)	0.6059(2)	0.0228(2)	0.042(2)	0.042(2)	0.034(2)	0.001(1)	–0.006(1)	0.009(2)
C(14)	4*e*	0.5407(2)	0.2017(2)	0.4941(2)	0.053(2)	0.044(2)	0.034(2)	0.002(1)	0.001(2)	–0.017(2)
C(15)	4*e*	0.4586(2)	0.2340(2)	0.4232(2)	0.045(2)	0.035(2)	0.044(2)	0.008(1)	0.007(2)	–0.009(2)
C(16)	4*e*	0.5392(2)	0.0948(2)	0.3186(2)	0.026(1)	0.030(1)	0.027(2)	–0.003(1)	0.004(1)	–0.007(1)
C(17)	4*e*	0.5405(2)	0.0614(2)	0.2138(2)	0.036(2)	0.022(1)	0.036(2)	–0.002(1)	0.005(1)	–0.001(1)
O(6)	4*e*	0.6992(1)	0.4847(1)	0.4924(1)	0.057(1)	0.067(1)	0.040(1)	–0.001(1)	0.004(1)	0.011(1)

References

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