Crystal structure of diisonicotinatotetraaquamanganese(II), $[Mn(C_5H_4NCOO)_2(H_2O)_4]$

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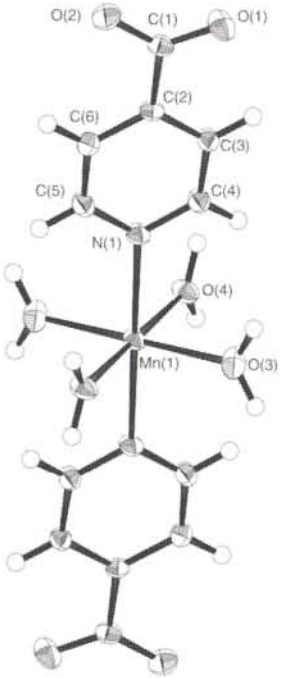

Abstract

$C_{12}H_{16}MnN_2O_8$, triclinic, $P\bar{1}$ (No. 2), $a = 6.3973(6)$ Å, $b = 6.941(1)$ Å, $c = 9.336(1)$ Å, $\alpha = 95.527(6)°$, $\beta = 104.386(2)°$, $\gamma = 112.518(2)°$, $V = 362.4$ Å^3, $Z = 1$, $R_{gt}(F) = 0.041$, $wR_{gt}(F) = 0.063$, $T = 273$ K.

Source of material

An aqueous solution (1 ml) of sodium isonicotinate (0.2 mmol) was transferred to a test tube, then an methanolic solution (1 ml) of manganese(II) chloride (0.1 mmol) was poured into the tube without mixing the two solutions. Large colourless crystals were obtained after one week.

Discussion

The reaction of sodium isonicotinate with manganese chloride affords a mononuclear complex $[Mn(H_2O)_4(C_5H_4NCOO)_2]$. The manganese centres are coordinated by four oxygen and two nitrogen atoms in a slightly distorted octahedral manner. Interestingly the isonicotinate ligand is only coordinating via the pyridyl nitrogen atoms and not via the carboxylate group. The $[Mn(H_2O)_4(C_5H_4NCOO)_2]$ molecule has a crystallographically imposed centre of inversion. The Mn—O bond lengths are 2.170(1) Å and 2.211(2) Å, respectively, whereas the Mn—N distance is 2.273(2) Å. The acute O–Mn–O angles are 86.18(8)° and 93.82(8)°, whereas the O–Mn–N angles range from 87.08(6)° to 92.92(6)°. The organic ligand has its expected geometry.

Table 1. Data collection and handling.

Crystal:	colourless column, size 0.20 × 0.21 × 0.36 mm
Wavelength:	Mo K_α radiation (0.7107 Å)
μ:	9.50 cm^{-1}
Diffractometer, scan mode:	Rigaku CCD, ω
$2\theta_{max}$:	55.2°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	1398, 1398
Criterion for F_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 3\ \sigma(I_{obs})$, 1329
$N(param)_{refined}$:	106
Programs:	teXsan [1], SIR92 [2]

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

Atom	Site	x	y	z	U_{iso}
H(1)	2*i*	0.7645	0.2878	0.4145	0.0230
H(2)	2*i*	1.0007	0.3980	0.6689	0.0258
H(3)	2*i*	0.4400	0.2936	0.8063	0.0286
H(4)	2*i*	0.1869	0.1711	0.5580	0.0249
H(5)	2*i*	1.1701	0.7503	0.8000	0.0382
H(6)	2*i*	1.3646	0.8647	0.9696	0.0382
H(7)	2*i*	1.1053	0.1924	0.8595	0.0286
H(8)	2*i*	1.2955	0.2889	1.0316	0.0286

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)	1*c*	1.0	1/2	1.0	0.0180(3)	0.0282(3)	0.0118(3)	0.0106(2)	0.0027(2)	0.0025(2)
O(1)	2*i*	0.3967(3)	0.2028(3)	0.1977(2)	0.0285(8)	0.059(1)	0.0182(9)	0.0229(8)	0.0058(7)	0.0108(7)
O(2)	2*i*	0.0731(3)	0.0792(3)	0.2711(2)	0.0209(7)	0.041(1)	0.024(1)	0.0088(7)	–0.0007(7)	0.0036(7)

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Table 3. Continued.

Atom	Site	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O(3)	2*i*	1.2216(3)	0.7537(3)	0.9058(2)	0.0270(8)	0.0392(9)	0.036(1)	0.0130(7)	0.0145(7)	0.0136(7)
O(4)	2*i*	1.1642(3)	0.2886(3)	0.9556(2)	0.0259(7)	0.0343(9)	0.0185(8)	0.0170(6)	0.0037(6)	0.0020(6)
N(1)	2*i*	0.7436(3)	0.3569(3)	0.7609(2)	0.0212(8)	0.0287(9)	0.0132(9)	0.0102(7)	0.0022(7)	0.0028(6)
C(1)	2*i*	0.2938(4)	0.1631(3)	0.2964(2)	0.024(1)	0.024(1)	0.017(1)	0.0123(8)	0.0022(8)	0.0024(7)
C(2)	2*i*	0.4503(3)	0.2259(3)	0.4597(2)	0.0196(9)	0.0172(9)	0.015(1)	0.0084(7)	0.0023(8)	0.0026(7)
C(3)	2*i*	0.6954(4)	0.2900(3)	0.4961(2)	0.020(1)	0.027(1)	0.016(1)	0.0083(8)	0.0061(8)	0.0052(7)
C(4)	2*i*	0.8331(4)	0.3531(4)	0.6459(2)	0.0181(9)	0.032(1)	0.019(1)	0.0102(8)	0.0054(8)	0.0045(8)
C(5)	2*i*	0.5061(4)	0.2898(4)	0.7252(3)	0.024(1)	0.036(1)	0.019(1)	0.0106(9)	0.0087(9)	0.0033(8)

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