Crystal structure of bis(1,3-diaminepropane)carbonatomanganese(III) chloride monohydrate, $[Mn(C_3H_{10}N_2)_2(CO_3)]Cl \cdot H_2O$

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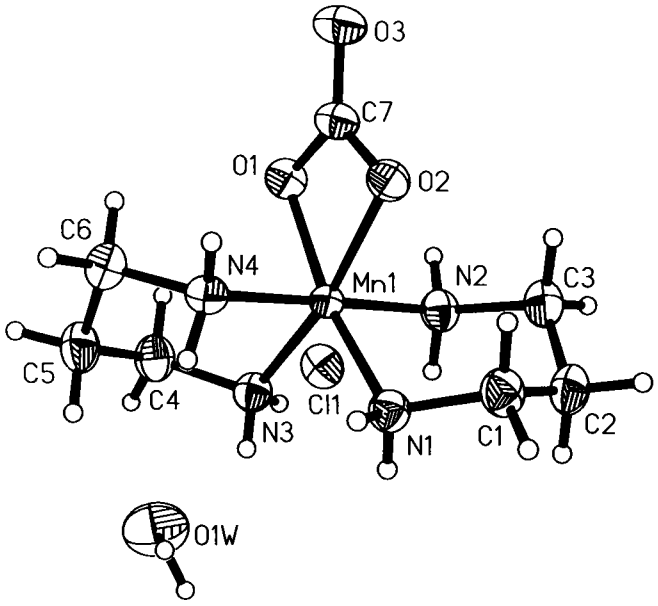
Received July 25, 2006, accepted and available on-line September 12, 2006; CCDC no. 1267/1852



Abstract

$C_7H_{22}ClMnN_4O_4$, monoclinic, $P12_1/n1$ (no. 14), $a = 8.997(2)$ Å, $b = 6.781(2)$ Å, $c = 21.398(6)$ Å, $\beta = 91.81(1)°$, $V = 1304.8$ Å^3, $Z = 4$, $R_{gt}(F) = 0.047$, $wR_{ref}(F^2) = 0.132$, $T = 293$ K.

Source of material

The title compound was prepared similarly to the procedure already reported [1]. $MnCl_2 \cdot 6H_2O$ and two equimolar amount 1,3-diaminopropane were dissolved in water and stirred for 1 h, during which the solution slowly changed from pale pink to dark violet. The mixed solution was stood in air for two weeks and filtered. The crystals obtained were washed with water, ethanol and diethyl ether, successively, and dried in air overnight (yield 48 %).

Discussion

Metal complexes with various organic ligands-containing nitrogen atoms have been a hot topics in the field of coordination chemistry [2-5]. Manganese element exists in some native enzymes and is required by creatures. Due to their biological relevant important behaviors, many manganese complexes with polyamine ligands have been reported in recent years [6-8].

The title crystal structure consists of one mononuclear complex cation, one chloride anion and one lattice water molecule. In the cation, the central manganese(III) atom is six-coordinated by four nitrogen atoms from two 1,3-diaminopropane molecules and by two nitrogen atoms from a carbonate anion. Both the amine and the carbonate group are bidentate ligands. The manganese atom is in a distorted octahedral environment, and the Mn—O and Mn—N bond lengths are in normal range. All the oxygen atoms both of the water and the carbonate anions, and all the nitrogen atoms participate to form hydrogen bonds, which join the constituents into a three-dimensional structure.

Table 1. Data collection and handling.

Crystal:	violet prism, size 0.25 × 0.32 × 0.41 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	12.26 cm^{-1}
Diffractometer, scan mode:	Siemens SMART CCD, φ/ω
$2\theta_{max}$:	49.92°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	2428, 2275
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 1818
$N(param)_{refined}$:	155
Program:	SHELXTL [9]

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

Atom	Site	x	y	z	U_{iso}
H(1NA)	4e	0.4850	0.3962	0.1437	0.08
H(1NB)	4e	0.5259	0.3805	0.0772	0.08
H(2NA)	4e	0.3817	−0.1154	0.1907	0.08
H(2NB)	4e	0.3974	0.1032	0.2152	0.08
H(3NA)	4e	0.2257	0.3793	0.1434	0.08
H(3NB)	4e	0.1945	0.2385	0.1788	0.08
H(4NA)	4e	0.3104	0.3485	0.0223	0.08
H(4NB)	4e	0.3545	0.1617	−0.0096	0.08
H(1A)	4e	0.7343	0.3576	0.1235	0.08
H(1B)	4e	0.6917	0.1517	0.0958	0.08
H(2A)	4e	0.7810	0.1223	0.1992	0.08
H(2B)	4e	0.6500	0.2515	0.2215	0.08
H(3A)	4e	0.6192	−0.1249	0.1677	0.08
H(3B)	4e	0.6037	−0.0850	0.2390	0.08
H(4A)	4e	−0.0110	0.3080	0.1361	0.08
H(4B)	4e	0.0348	0.0998	0.1126	0.08
H(5A)	4e	−0.0492	0.2998	0.0305	0.08
H(5B)	4e	0.0820	0.4429	0.0452	0.08
H(6A)	4e	0.1225	0.0590	0.0038	0.08
H(6B)	4e	0.1350	0.2426	−0.0399	0.08
H(1WA)	4e	0.0413	0.7945	0.1956	0.08
H(1WB)	4e	0.1020	0.7635	0.1339	0.08

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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)	4e	0.36523(6)	0.11113(8)	0.10449(2)	0.0310(3)	0.0322(3)	0.0303(3)	–0.0001(2)	0.0049(2)	–0.0002(2)
N(1)	4e	0.5131(4)	0.3159(6)	0.1126(2)	0.045(2)	0.052(2)	0.048(2)	0.001(2)	0.002(2)	–0.001(2)
N(2)	4e	0.4282(4)	0.0095(6)	0.1865(2)	0.042(2)	0.057(2)	0.048(2)	0.003(2)	0.006(2)	0.002(2)
N(3)	4e	0.2095(4)	0.2622(5)	0.1414(2)	0.046(2)	0.052(2)	0.044(2)	0.001(2)	0.002(2)	–0.001(2)
N(4)	4e	0.3076(4)	0.2185(5)	0.0230(2)	0.048(2)	0.042(2)	0.044(2)	–0.000(2)	0.005(2)	–0.002(2)
O(1)	4e	0.2549(3)	–0.1238(4)	0.0876(1)	0.048(2)	0.049(2)	0.050(2)	0.000(1)	0.008(1)	0.001(1)
O(2)	4e	0.4812(3)	–0.0831(4)	0.0655(1)	0.047(2)	0.049(2)	0.049(2)	0.003(1)	0.007(1)	–0.001(1)
O(3)	4e	0.3715(4)	–0.3630(5)	0.0353(2)	0.084(2)	0.044(2)	0.076(2)	0.002(2)	0.005(2)	–0.010(2)
C(1)	4e	0.6667(5)	0.2485(7)	0.1267(2)	0.042(2)	0.062(3)	0.068(3)	–0.001(2)	0.005(2)	0.003(2)
C(2)	4e	0.6788(5)	0.1562(8)	0.1907(3)	0.042(2)	0.078(3)	0.067(3)	0.001(2)	–0.005(2)	–0.001(3)
C(3)	4e	0.5881(5)	–0.0290(8)	0.1979(2)	0.050(3)	0.068(3)	0.056(3)	0.007(2)	–0.002(2)	0.003(2)
C(4)	4e	0.0603(5)	0.2378(8)	0.1119(2)	0.046(2)	0.068(3)	0.060(3)	0.002(2)	0.003(2)	0.006(2)
C(5)	4e	0.0520(5)	0.3066(8)	0.0459(2)	0.047(3)	0.077(3)	0.059(3)	0.011(3)	–0.001(2)	0.003(3)
C(6)	4e	0.1495(5)	0.1964(8)	0.0025(2)	0.050(2)	0.061(3)	0.049(3)	–0.004(2)	–0.001(2)	0.003(2)
C(7)	4e	0.3684(5)	–0.2027(6)	0.0611(2)	0.058(3)	0.038(2)	0.049(3)	0.001(2)	0.006(2)	–0.002(2)
O(1W)	4e	0.0218(5)	0.7065(7)	0.1584(2)	0.116(4)	0.092(3)	0.110(4)	–0.032(3)	0.026(3)	0.006(3)
Cl(1)	4e	0.0983(2)	0.0443(2)	0.26487(6)	0.0728(8)	0.0675(8)	0.0529(7)	0.0036(6)	0.0103(6)	0.0115(6)

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