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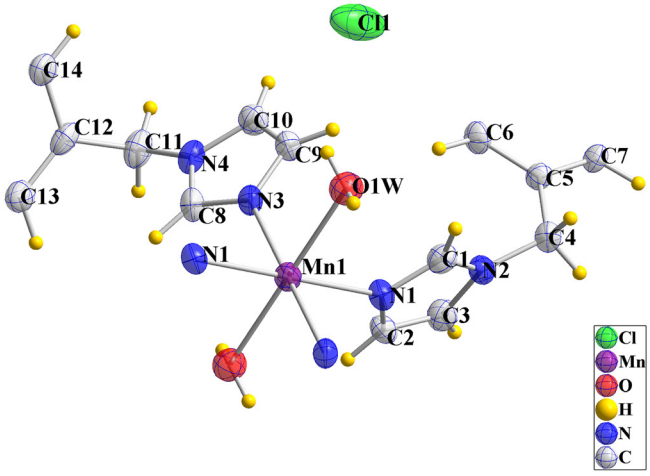
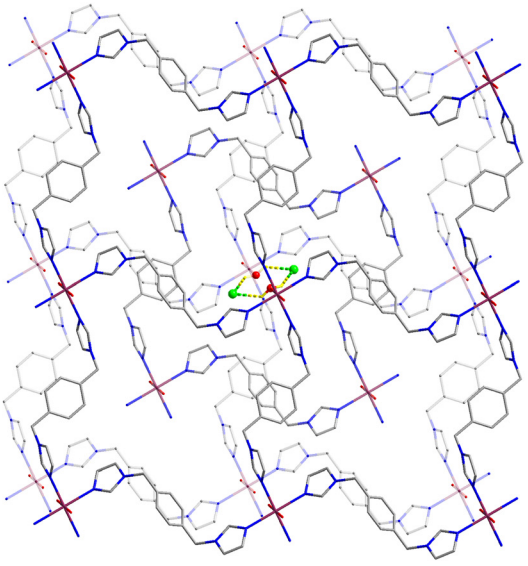
Crystal structure of poly[diaqua-(bis(m$_2$-1,4-bis(imidazol-1-ylmethyl)benzene)-κ^2N,N'-manganese] dichloride, $C_{28}H_{32}MnN_8O_2Cl_2$





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Abstract

$C_{28}H_{32}MnN_8O_2Cl_2$, triclinic, $P\bar{1}$ (no. 2), a = 8.987(4) Å, b = 9.061(3) Å, c = 10.706(2) Å, α = 88.65(2)°, β = 66.12(2)°, γ = 89.89(2)°, V = 796.9(5) Å^3, Z = 1, $R_{gt}(F)$ = 0.1033, w$R_{ref}(F^2)$ = 0.2218, T = 293(2) K.

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

Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.32 × 0.28 × 0.21 mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ:	0.62 mm^{-1}
Diffractometer, scan mode:	φ and ω
θ_{max}, completeness:	25.0°, 98 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	3982, 2745, 0.070
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 1128
$N(param)_{refined}$:	194
Programs:	Bruker [1], Olex2 [2], SHELX [3]

1 Source of materials

The 2,2-dimethylsuccinic acid (0.044 g, 0.3 mmol), 1,4-bis(imidazol-1-ylmethyl)benzene (0.071 g, 0.3 mmol) and $MnCl_2{\cdot}2H_2O$ (0.048 g, 0.3 mmol) were dissolved in deionized water (8 mL). The mixture was stirred rigorously and transferred into a 23 mL teflon-lined stainless-steel vessel, which was followed by heating at 140 °C under autogenous pressure for two days. After the mixture was cooled to room temperature, pale yellow block crystals were obtained, washed with ethanol, and dried at room temperature.

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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}
Cl1	0.5990 (4)	0.5964 (5)	0.2963 (4)	0.1405 (18)
Mn1	0.0000	0.5000	0.5000	0.0519 (7)
O1W	0.2480 (8)	0.5021 (8)	0.4997 (7)	0.072 (2)
H1WA	0.233 (3)	0.508 (11)	0.579 (2)	0.108*
H1WB	0.302 (4)	0.554 (9)	0.436 (6)	0.108*
N1	0.0357 (9)	0.2699 (8)	0.4355 (7)	0.052 (2)
N2	0.1690 (9)	0.0689 (8)	0.3426 (7)	0.0514 (19)
N3	0.1052 (9)	0.5628 (7)	0.2770 (8)	0.054 (2)
N4	0.1195 (10)	0.6317 (7)	0.0727 (8)	0.055 (2)
C1	0.1675 (12)	0.1909 (10)	0.4113 (9)	0.056 (2)
H1A	0.2495	0.2168	0.4388	0.068*
C2	−0.0469 (11)	0.1936 (11)	0.3756 (9)	0.056 (2)
H2A	−0.1462	0.2229	0.3756	0.067*
C3	0.0296 (12)	0.0743 (11)	0.3181 (9)	0.062 (3)
H3A	−0.0033	0.0065	0.2703	0.075*
C4	0.2950 (11)	−0.0380 (10)	0.2913 (10)	0.064 (3)
H4A	0.2462	−0.1358	0.3071	0.077*
H4B	0.3635	−0.0327	0.3416	0.077*
C5	0.3997 (10)	−0.0160 (9)	0.1401 (8)	0.045 (2)
C6	0.4213 (11)	0.1170 (10)	0.0728 (9)	0.056 (2)
H6	0.3684	0.1991	0.1213	0.067*
C7	0.4807 (10)	−0.1346 (9)	0.0653 (9)	0.051 (2)
H7	0.4697	−0.2271	0.1077	0.062*
C8	0.0332 (12)	0.6342 (10)	0.2089 (11)	0.061 (3)
H8A	−0.0664	0.6812	0.2502	0.073*
C9	0.2460 (11)	0.5129 (10)	0.1765 (10)	0.058 (3)
H9A	0.3242	0.4574	0.1921	0.070*
C10	0.2552 (12)	0.5545 (10)	0.0550 (10)	0.061 (3)
H10A	0.3399	0.5344	−0.0283	0.073*
C11	0.0747 (14)	0.6927 (10)	−0.0331 (10)	0.072 (3)
H11A	−0.0184	0.6385	−0.0330	0.087*
H11B	0.1642	0.6803	−0.1213	0.087*
C12	0.0335 (13)	0.8529 (10)	−0.0143 (10)	0.057 (3)
C13	−0.1243 (13)	0.8991 (12)	0.0606 (10)	0.067 (3)
H13	−0.2070	0.8296	0.1013	0.081*
C14	0.1587 (13)	0.9535 (11)	−0.0748 (10)	0.066 (3)
H14	0.2645	0.9218	−0.1243	0.080*

2 Experimental details

The H atoms bonded to carbon were generated according to their calculated positions, while the water hydrogen atoms were located from difference Fourier maps and refined isotropically with their U_{iso} values of $1.5U_{eq}$(C).

3 Comment

For the past few decades, bis(imidazole) molecules have been demonstrated to be effective bridging ligands for the construction of the coordination polymers with intriguing topologies and special functionality in photoluminescence, catalysis, magnetics, and so on [4–9].

Crystal structure analysis reveals that the asymmetric unit is composed of one central Mn(II) atom, two halves bix ligands, one coordinated water molecule and one chloride anion. The central Mn(II) atom adopts typical six-coordinated octahedral geometry surrounded by four imidazole nitrogen atoms in the equatorial plane and two water oxygen atoms in axial positions. Mn–N bond lengths are between 2.194(7) and 2.242(7) Å, while the Mn–O bond length is 2.228(7) Å, which is in agreement with the reported Mn–N and Mn–O bond lengths [10–12]. The neutral 1,4-bis(imidazol-1-ylmethyl)benzene molecule adopts two kinds of *trans* conformations to interconnect Mn(II) atoms with neighboring distances of 13.862 and 14.277 Å, resulting into a 2D 4^4-sql layer. The free chloride anions serve as the counter ions for the electropositive layers to be positioned in the lattice enclosed by the bix–Mn(II) host layer, which is sandwiched between the two adjacent layers with the electrostatic attraction and O–H···Cl hydrogen interaction, thus reinforcing the supramolecular framework.

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