Crystal structure of metaclopromidemanganese chloride complex, $C_{32}H_{44}Cl_2MnN_{10}O_4S_4$

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Fig. 1. ORTEP plot of the molecules.

Source of material: see ref. 1.

The bond distances and angles do not show any large deviations. The thermal ellipsoid plot of the molecule is shown in Fig. 1. The packing of the molecules down *b* is shown in Fig. 2. The metal and the ligands are stacked in separate layers.

$C_{32}H_{44}Cl_2MnN_{10}O_4S_4$, orthorhombic, $Pna2_1$ (No. 33), $a = 16.538(2)$ Å, $b = 12.143(2)$ Å, $c = 21.610(3)$ Å, $V = 4339.7$ Å³, $Z = 4$, $R(F) = 0.038$, $R_w(F^2) = 0.110$.

Fig. 2. Packing of molecules down *b*.

Table 1. Parameters used for the X-ray data collection

Crystal:	green, rectangular, size 0.20 x 0.35 x 0.35 mm
Wavelength:	Mo $K\alpha$ radiation (0.71069 Å)
μ :	6.66 cm ⁻¹
Diffractometer:	Rigaku AFC7S
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	50°
$N(hkl)_{\text{unique}}$:	3931
Criterion for I_o :	$I_o > 2 \sigma(I_o)$
$N(\text{param})_{\text{refined}}$:	485
Programs:	SHELXS-86, SHELXL-93

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
C(1')	4a	-0.2576(4)	-0.4093(5)	1.0883(4)	0.059(4)	0.041(3)	0.065(4)	-0.001(3)	0.017(3)	0.002(3)
C(2')	4a	-0.2866(5)	-0.3810(6)	1.0307(4)	0.073(5)	0.054(4)	0.085(6)	-0.001(4)	0.015(4)	0.011(4)
C(3')	4a	-0.2702(5)	-0.2807(8)	1.0043(5)	0.074(5)	0.075(5)	0.109(7)	0.015(4)	0.025(5)	0.038(5)
C(4')	4a	-0.2231(6)	-0.2025(7)	1.0338(6)	0.079(5)	0.051(4)	0.130(9)	0.003(4)	0.036(6)	0.026(5)
C(5')	4a	-0.1950(6)	-0.2288(7)	1.0931(6)	0.091(6)	0.046(4)	0.128(8)	-0.012(4)	0.045(6)	-0.007(5)
C(6')	4a	-0.2108(5)	-0.3300(6)	1.1206(4)	0.076(5)	0.041(3)	0.086(5)	-0.008(3)	0.025(4)	-0.011(4)
Cl(7')	4a	-0.3086(3)	-0.2496(3)	0.9314(2)	0.149(3)	0.142(3)	0.147(3)	0.010(2)	0.000(2)	0.089(3)
N(8')	4a	-0.2063(6)	-0.1028(7)	1.0071(6)	0.122(8)	0.063(5)	0.20(1)	-0.006(5)	0.037(7)	0.050(6)
O(9')	4a	-0.1844(4)	-0.3593(5)	1.1777(3)	0.108(4)	0.065(3)	0.086(4)	-0.040(3)	0.010(4)	-0.009(3)
C(10')	4a	-0.1360(8)	-0.282(1)	1.2134(6)	0.114(8)	0.101(7)	0.114(8)	-0.062(7)	0.003(7)	-0.022(7)
O(11')	4a	-0.3026(3)	-0.5920(4)	1.0733(2)	0.075(3)	0.050(2)	0.061(3)	-0.007(2)	0.005(2)	-0.004(2)
C(12')	4a	-0.2777(4)	-0.5214(5)	1.1104(3)	0.054(3)	0.039(3)	0.059(4)	-0.002(3)	0.008(3)	-0.001(3)

Table 2. (Continued)

Atom	Site	x	y	z	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
N(13')	4a	-0.2702(4)	-0.5454(4)	1.1704(3)	0.073(4)	0.040(3)	0.060(3)	-0.013(3)	0.000(3)	0.001(2)
C(14')	4a	-0.2911(4)	-0.6548(5)	1.1941(4)	0.067(4)	0.038(3)	0.065(4)	-0.004(3)	-0.002(3)	0.011(3)
C(15')	4a	-0.3821(4)	-0.6612(5)	1.2017(3)	0.066(4)	0.042(3)	0.057(4)	0.004(3)	0.009(3)	0.010(3)
N(16')	4a	-0.4117(3)	-0.7760(4)	1.2139(3)	0.056(3)	0.044(3)	0.057(3)	-0.005(2)	0.004(3)	0.006(2)
C(17')	4a	-0.3764(5)	-0.8274(6)	1.2709(4)	0.085(5)	0.054(4)	0.070(5)	-0.013(4)	0.004(4)	0.020(4)
C(18')	4a	-0.393(1)	-0.7660(9)	1.3299(4)	0.20(1)	0.086(6)	0.051(4)	-0.027(7)	0.009(6)	0.004(4)
C(19')	4a	-0.5025(5)	-0.7785(8)	1.2113(5)	0.054(4)	0.076(6)	0.107(7)	0.001(4)	0.000(4)	0.000(5)
C(20')	4a	-0.5377(6)	-0.8913(9)	1.2092(6)	0.068(5)	0.094(7)	0.123(8)	-0.020(5)	-0.008(6)	0.014(6)
C(1)	4a	-0.3948(4)	-0.0604(5)	1.1020(3)	0.056(3)	0.047(3)	0.047(3)	-0.006(3)	0.005(3)	0.001(3)
C(2)	4a	-0.3662(4)	-0.0867(6)	1.1603(3)	0.058(4)	0.050(4)	0.059(4)	-0.002(3)	0.004(3)	0.000(3)
C(3)	4a	-0.3808(4)	-0.1873(6)	1.1862(4)	0.056(4)	0.061(4)	0.068(5)	0.009(3)	0.011(3)	0.016(4)
C(4)	4a	-0.4263(5)	-0.2666(6)	1.1558(4)	0.064(4)	0.052(4)	0.080(5)	0.005(3)	0.023(4)	0.019(4)
C(5)	4a	-0.4559(5)	-0.2408(6)	1.0976(4)	0.086(5)	0.051(4)	0.067(4)	-0.018(4)	0.015(4)	-0.002(3)
C(6)	4a	-0.4408(5)	-0.1377(6)	1.0708(3)	0.073(4)	0.060(4)	0.051(4)	-0.015(3)	0.004(3)	0.002(3)
Cl(7)	4a	-0.3420(2)	-0.2180(3)	1.2596(1)	0.109(2)	0.115(2)	0.085(2)	0.004(2)	-0.010(1)	0.044(2)
N(8)	4a	-0.4423(5)	-0.3675(6)	1.1825(4)	0.101(5)	0.058(4)	0.111(6)	-0.001(4)	0.017(5)	0.028(4)
O(9)	4a	-0.4697(5)	-0.1105(5)	1.0142(3)	0.133(6)	0.078(4)	0.065(3)	-0.062(4)	-0.026(4)	0.010(3)
C(10)	4a	-0.521(1)	-0.186(1)	0.9826(6)	0.21(2)	0.15(1)	0.092(8)	-0.13(1)	-0.060(9)	0.033(8)
O(11)	4a	-0.3478(3)	0.1227(4)	1.1152(2)	0.082(3)	0.048(2)	0.052(3)	-0.014(2)	0.001(2)	-0.007(2)
C(12)	4a	-0.3747(4)	0.0517(5)	1.0785(3)	0.053(3)	0.040(3)	0.054(4)	-0.005(3)	0.005(3)	-0.004(3)
N(13)	4a	-0.3814(4)	0.0760(5)	1.0188(3)	0.088(4)	0.047(3)	0.054(3)	-0.023(3)	-0.009(3)	0.002(3)
C(14)	4a	-0.3577(5)	0.1828(6)	0.9959(4)	0.078(5)	0.049(4)	0.065(4)	-0.014(3)	-0.017(4)	0.013(3)
C(15)	4a	-0.2656(4)	0.1877(6)	0.9909(3)	0.074(4)	0.052(4)	0.049(3)	0.000(3)	0.005(3)	0.005(3)
N(16)	4a	-0.2341(4)	0.3001(5)	0.9741(3)	0.064(3)	0.056(3)	0.056(3)	-0.008(3)	0.009(3)	0.006(3)
C(17)	4a	-0.2626(7)	0.3322(8)	0.9093(4)	0.114(7)	0.093(6)	0.064(5)	-0.024(6)	0.003(5)	0.022(5)
C(18)	4a	-0.2421(7)	0.4443(8)	0.8897(5)	0.115(8)	0.088(6)	0.086(6)	0.009(6)	0.011(6)	0.027(5)
C(19)	4a	-0.1432(6)	0.3026(9)	0.9794(6)	0.070(6)	0.088(6)	0.121(9)	-0.003(5)	0.031(6)	0.022(6)
C(20)	4a	-0.1152(7)	0.332(1)	1.0415(8)	0.074(7)	0.19(1)	0.16(1)	0.010(8)	-0.027(8)	-0.03(1)
N(21)	4a	0.0735(6)	-0.0046(7)	0.7944(4)	0.113(7)	0.091(6)	0.096(6)	0.006(5)	0.005(5)	-0.017(5)
C(22)	4a	0.1157(5)	-0.0323(7)	0.7549(4)	0.072(5)	0.055(4)	0.076(5)	-0.006(4)	-0.003(4)	-0.005(4)
S(23)	4a	0.1732(2)	-0.0703(2)	0.7000(1)	0.079(1)	0.094(2)	0.096(2)	-0.008(1)	0.015(1)	-0.012(1)
N(24)	4a	-0.1136(6)	0.0393(7)	0.8437(5)	0.089(5)	0.081(5)	0.131(8)	-0.006(4)	-0.025(6)	-0.005(5)
C(25)	4a	-0.1808(6)	0.0282(6)	0.8407(4)	0.090(6)	0.048(4)	0.065(4)	0.004(4)	-0.001(4)	-0.002(3)
S(26)	4a	-0.2782(1)	0.0133(2)	0.8377(1)	0.077(1)	0.085(1)	0.088(1)	-0.001(1)	0.001(1)	-0.001(1)
N(27)	4a	0.0203(5)	0.2400(6)	0.8570(5)	0.086(5)	0.066(4)	0.100(6)	-0.001(3)	-0.008(5)	-0.003(4)
C(28)	4a	0.0131(4)	0.3331(7)	0.8609(4)	0.055(4)	0.073(5)	0.060(4)	-0.004(3)	-0.002(4)	0.007(4)
S(29)	4a	0.0050(2)	0.4644(2)	0.8702(2)	0.097(2)	0.066(1)	0.103(2)	0.005(1)	0.005(1)	0.004(1)
N(30)	4a	0.0267(6)	0.0333(8)	0.9515(5)	0.106(6)	0.101(6)	0.082(6)	0.007(5)	0.001(5)	0.003(5)
C(31)	4a	0.0013(6)	0.0369(8)	1.0007(5)	0.082(6)	0.070(5)	0.088(7)	0.007(4)	-0.017(5)	0.006(5)
S(32)	4a	-0.0369(2)	0.0429(3)	1.0698(1)	0.124(2)	0.098(2)	0.084(2)	0.012(2)	0.005(2)	0.004(1)
Mn	4a	0.00582(8)	0.0728(1)	0.86069(7)	0.0752(7)	0.0677(7)	0.0786(8)	0.0026(5)	0.0000(7)	-0.0104(7)

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