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[MnTPClPP][TCNE]·2PhMe

Table S1. Crystal data and structure refinement for 1.

Identification code	shelxs
Empirical formula	C64 H40 Cl4 Mn N8
Formula weight	1117.78
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a = 10.171(4) A alpha = 107.51(2) deg. b = 10.189(3) A beta = 85.58(2) deg. c = 14.522(3) A gamma = 111.51(3) deg.
Volume	1334.4(7) A^3
Z	1
Density (calculated)	1.391 Mg/m^3
Absorption coefficient	0.498 mm^-1
F(000)	573
Crystal size	0.22 x 0.19 x 0.03 mm
Theta range for data collection	2.15 to 23.97 deg.
Index ranges	0<=h<=11, -11<=k<=10, -16<=l<=16
Reflections collected	4441
Independent reflections	4176 [R(int) = 0.0328]
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.999 and 0.906
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4176 / 0 / 350
Goodness-of-fit on F^2	1.036
Final R indices [I>2sigma(I)]	R1 = 0.0426, wR2 = 0.0831
R indices (all data)	R1 = 0.0902, wR2 = 0.0981

[MnTPClPP][TCNE]·2PhMe

Largest diff. peak and hole	0.330 and -0.297 e.A^-3

[MnTPClPP][TCNE]·2PhMe

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 1. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mn	0	0	5000	21(1)
Cl(1)	9080(1)	3400(1)	2575(1)	59(1)
Cl(2)	3642(1)	3768(1)	1448(1)	71(1)
N(1)	-478(3)	2081(3)	5239(2)	33(1)
N(2)	-2584(3)	5348(3)	5989(2)	49(1)
N(3)	1922(3)	1214(3)	5661(2)	23(1)
N(4)	807(3)	200(3)	3724(2)	23(1)
C(1)	-532(3)	3180(4)	5234(2)	27(1)
C(2)	-551(3)	4541(3)	5211(2)	26(1)
C(3)	-1682(4)	4981(4)	5640(3)	30(1)
C(4)	3176(3)	1743(3)	5213(2)	26(1)
C(5)	4303(3)	2521(3)	5925(2)	30(1)
C(6)	3747(3)	2464(4)	6787(2)	30(1)
C(7)	2261(3)	1649(3)	6634(2)	25(1)
C(8)	1325(3)	1281(3)	7348(2)	26(1)
C(9)	91(3)	-400(3)	2833(2)	27(1)
C(10)	1078(4)	-32(4)	2108(2)	32(1)
C(11)	2362(4)	752(4)	2541(2)	31(1)
C(12)	2212(3)	891(3)	3547(2)	24(1)
C(13)	3328(3)	1579(3)	4234(2)	24(1)
C(14)	4790(3)	2105(3)	3872(2)	26(1)
C(15)	5333(4)	3396(4)	3608(3)	38(1)
C(16)	6657(4)	3809(4)	3219(3)	43(1)
C(17)	7431(3)	2924(4)	3096(2)	37(1)
C(18)	6938(4)	1657(4)	3367(3)	42(1)
C(19)	5621(4)	1260(4)	3761(3)	38(1)
C(20)	1900(3)	1889(4)	8374(2)	28(1)
C(21)	2440(3)	3410(4)	8814(2)	33(1)
C(22)	2981(4)	3990(4)	9754(2)	38(1)
C(23)	2959(4)	3044(4)	10264(2)	39(1)
C(24)	2424(4)	1535(4)	9852(3)	39(1)
C(25)	1901(4)	969(4)	8908(2)	33(1)
C(26)	7654(5)	2950(5)	7444(3)	69(1)
C(27)	7475(4)	2725(4)	8430(3)	45(1)
C(28)	6164(4)	1961(4)	8715(3)	48(1)
C(29)	6010(5)	1715(5)	9611(3)	57(1)
C(30)	7166(5)	2223(5)	10220(3)	61(1)
C(31)	8469(5)	2996(5)	9954(3)	63(1)
C(32)	8623(4)	3242(4)	9065(3)	54(1)

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Table S3. Bond lengths [Å] and angles [deg] for 1.

Mn-N(4)	2.005(3)
Mn-N(3)	2.018(3)
Mn-N(1)	2.267(3)
Cl(1)-C(17)	1.747(3)
Cl(2)-C(23)#2	1.739(3)
N(1)-C(1)	1.144(4)
N(2)-C(3)	1.142(4)
N(3)-C(7)	1.378(4)
N(3)-C(4)	1.386(4)
N(4)-C(12)	1.385(4)
N(4)-C(9)	1.385(4)
C(1)-C(2)	1.404(4)
C(2)-C(2)#3	1.406(6)
C(2)-C(3)	1.418(5)
C(4)-C(13)	1.385(4)
C(4)-C(5)	1.426(4)
C(5)-C(6)	1.343(4)
C(6)-C(7)	1.430(4)
C(7)-C(8)	1.394(4)
C(8)-C(9)#1	1.385(4)
C(8)-C(20)	1.503(4)
C(9)-C(10)	1.434(4)
C(10)-C(11)	1.341(4)
C(11)-C(12)	1.427(4)
C(12)-C(13)	1.395(4)
C(13)-C(14)	1.496(4)
C(14)-C(19)	1.383(4)
C(14)-C(15)	1.385(4)
C(15)-C(16)	1.386(5)
C(16)-C(17)	1.366(5)
C(17)-C(18)	1.369(5)
C(18)-C(19)	1.382(5)
C(20)-C(25)	1.386(4)
C(20)-C(21)	1.395(4)
C(21)-C(22)	1.382(5)
C(22)-C(23)	1.375(5)
C(23)-C(24)	1.379(5)
C(24)-C(25)	1.380(5)
C(26)-C(27)	1.505(5)
C(27)-C(28)	1.379(5)
C(27)-C(32)	1.384(5)
C(28)-C(29)	1.385(5)
C(29)-C(30)	1.368(6)
C(30)-C(31)	1.366(6)
C(31)-C(32)	1.375(6)
N(4)#1-Mn-N(4)	180.0
N(4)-Mn-N(3)#1	89.60(10)
N(4)-Mn-N(3)	90.40(10)
N(3)#1-Mn-N(3)	180.0

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N(4)#1-Mn-N(1)	90.51(10)
N(4)-Mn-N(1)	89.49(10)
N(3)#1-Mn-N(1)	89.78(10)
N(3)-Mn-N(1)	90.22(10)
N(1)-Mn-N(1)#1	180.0
C(1)-N(1)-Mn	167.2(3)
C(7)-N(3)-C(4)	106.3(3)
C(7)-N(3)-Mn	127.4(2)
C(4)-N(3)-Mn	126.3(2)
C(12)-N(4)-C(9)	106.1(3)
C(12)-N(4)-Mn	126.7(2)
C(9)-N(4)-Mn	127.1(2)
N(1)-C(1)-C(2)	177.9(4)
C(1)-C(2)-C(2)#3	120.3(4)
C(1)-C(2)-C(3)	118.7(3)
C(2)#3-C(2)-C(3)	121.0(4)
N(2)-C(3)-C(2)	179.4(3)
C(13)-C(4)-N(3)	126.1(3)
C(13)-C(4)-C(5)	124.6(3)
N(3)-C(4)-C(5)	109.3(3)
C(6)-C(5)-C(4)	107.5(3)
C(5)-C(6)-C(7)	107.9(3)
N(3)-C(7)-C(8)	125.6(3)
N(3)-C(7)-C(6)	109.0(3)
C(8)-C(7)-C(6)	125.3(3)
C(9)#1-C(8)-C(7)	124.0(3)
C(9)#1-C(8)-C(20)	118.6(3)
C(7)-C(8)-C(20)	117.4(3)
N(4)-C(9)-C(8)#1	126.3(3)
N(4)-C(9)-C(10)	108.7(3)
C(8)#1-C(9)-C(10)	124.9(3)
C(11)-C(10)-C(9)	108.2(3)
C(10)-C(11)-C(12)	107.3(3)
N(4)-C(12)-C(13)	125.8(3)
N(4)-C(12)-C(11)	109.6(3)
C(13)-C(12)-C(11)	124.5(3)
C(4)-C(13)-C(12)	124.4(3)
C(4)-C(13)-C(14)	118.3(3)
C(12)-C(13)-C(14)	117.2(3)
C(19)-C(14)-C(15)	118.1(3)
C(19)-C(14)-C(13)	119.6(3)
C(15)-C(14)-C(13)	122.2(3)
C(14)-C(15)-C(16)	121.0(3)
C(17)-C(16)-C(15)	119.1(3)
C(16)-C(17)-C(18)	121.4(3)
C(16)-C(17)-Cl(1)	119.8(3)
C(18)-C(17)-Cl(1)	118.8(3)
C(17)-C(18)-C(19)	119.0(3)
C(18)-C(19)-C(14)	121.3(3)
C(25)-C(20)-C(21)	118.3(3)
C(25)-C(20)-C(8)	121.4(3)
C(21)-C(20)-C(8)	120.2(3)
C(22)-C(21)-C(20)	121.0(3)
C(23)-C(22)-C(21)	119.1(3)

C(22)-C(23)-C(24)	121.3(3)
C(22)-C(23)-Cl(2)#4	119.3(3)
C(24)-C(23)-Cl(2)#4	119.5(3)
C(23)-C(24)-C(25)	119.2(3)
C(24)-C(25)-C(20)	121.1(3)
C(28)-C(27)-C(32)	118.2(4)
C(28)-C(27)-C(26)	120.7(4)
C(32)-C(27)-C(26)	121.0(4)
C(27)-C(28)-C(29)	120.6(4)
C(30)-C(29)-C(28)	120.0(4)
C(31)-C(30)-C(29)	120.2(4)
C(30)-C(31)-C(32)	119.8(4)
C(31)-C(32)-C(27)	121.1(4)

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z+1 #2 x,y,z-1 #3 -x,-y+1,-z+1
#4 x,y,z+1

Table S4. Anisotropic displacement parameters (A^2 x 10^3) for 1. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mn	21(1)	19(1)	24(1)	9(1)	3(1)	6(1)
Cl(1)	26(1)	91(1)	39(1)	8(1)	9(1)	7(1)
Cl(2)	108(1)	57(1)	32(1)	9(1)	-23(1)	11(1)
N(1)	36(2)	27(2)	43(2)	15(1)	9(1)	15(1)
N(2)	36(2)	40(2)	73(3)	18(2)	13(2)	17(2)
N(3)	22(2)	22(1)	24(2)	10(1)	1(1)	5(1)
N(4)	22(2)	21(1)	26(2)	10(1)	3(1)	7(1)
C(1)	28(2)	27(2)	25(2)	9(2)	1(2)	9(2)
C(2)	28(2)	24(2)	30(2)	9(2)	0(2)	11(2)
C(3)	27(2)	23(2)	42(2)	15(2)	2(2)	6(2)
C(4)	24(2)	23(2)	33(2)	12(2)	5(2)	9(2)
C(5)	21(2)	30(2)	36(2)	13(2)	1(2)	2(2)
C(6)	27(2)	32(2)	30(2)	11(2)	-2(2)	7(2)
C(7)	25(2)	21(2)	28(2)	7(2)	-1(2)	8(2)
C(8)	28(2)	24(2)	26(2)	7(2)	-1(2)	9(2)
C(9)	32(2)	22(2)	26(2)	7(2)	1(2)	10(2)
C(10)	37(2)	37(2)	23(2)	12(2)	5(2)	13(2)
C(11)	30(2)	35(2)	30(2)	15(2)	7(2)	11(2)
C(12)	25(2)	23(2)	28(2)	12(2)	6(2)	8(2)
C(13)	22(2)	25(2)	27(2)	10(2)	3(2)	8(2)
C(14)	25(2)	27(2)	23(2)	6(2)	1(2)	6(2)
C(15)	30(2)	42(2)	47(2)	21(2)	7(2)	15(2)
C(16)	33(2)	51(2)	47(2)	29(2)	10(2)	8(2)
C(17)	17(2)	56(3)	27(2)	7(2)	3(2)	7(2)
C(18)	34(2)	46(2)	46(2)	6(2)	3(2)	20(2)
C(19)	32(2)	34(2)	49(2)	15(2)	7(2)	13(2)
C(20)	24(2)	32(2)	25(2)	8(2)	4(2)	9(2)
C(21)	36(2)	34(2)	30(2)	11(2)	-1(2)	13(2)
C(22)	44(2)	27(2)	35(2)	5(2)	-3(2)	7(2)
C(23)	47(2)	44(2)	23(2)	10(2)	-3(2)	11(2)
C(24)	46(2)	38(2)	32(2)	15(2)	-4(2)	8(2)
C(25)	35(2)	28(2)	32(2)	10(2)	1(2)	7(2)
C(26)	87(4)	65(3)	58(3)	25(2)	18(3)	29(3)
C(27)	49(3)	39(2)	48(3)	10(2)	7(2)	19(2)
C(28)	45(3)	43(2)	53(3)	13(2)	-8(2)	14(2)
C(29)	50(3)	54(3)	72(3)	29(2)	11(2)	17(2)
C(30)	80(4)	58(3)	50(3)	15(2)	-5(3)	29(3)
C(31)	63(3)	56(3)	63(3)	0(2)	-21(3)	24(3)
C(32)	41(2)	43(3)	69(3)	7(2)	0(2)	10(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 1.

	x	y	z	U(eq)
H(5)	5269(3)	2994(3)	5810(2)	36
H(6)	4252(3)	2889(4)	7393(2)	36
H(10)	860(4)	-297(4)	1437(2)	38
H(11)	3215(4)	1142(4)	2234(2)	37
H(15)	4790(4)	4007(4)	3696(3)	45
H(16)	7021(4)	4696(4)	3039(3)	51
H(18)	7493(4)	1059(4)	3285(3)	51
H(19)	5280(4)	389(4)	3959(3)	45
H(21)	2436(3)	4057(4)	8461(2)	39
H(22)	3362(4)	5028(4)	10045(2)	45
H(24)	2415(4)	893(4)	10212(3)	47
H(25)	1535(4)	-70(4)	8620(2)	39
H(26A)	8648(5)	3512(5)	7368(3)	103
H(26B)	7068(5)	3495(5)	7372(3)	103
H(26C)	7360(5)	1988(5)	6949(3)	103
H(26D)	6736(5)	2485(5)	7091(3)	103
H(26E)	8316(5)	2502(5)	7087(3)	103
H(26F)	8024(5)	4009(5)	7510(3)	103
H(28)	5360(4)	1600(4)	8292(3)	57
H(29)	5102(5)	1194(5)	9802(3)	69
H(30)	7061(5)	2038(5)	10830(3)	73
H(31)	9268(5)	3362(5)	10383(3)	75
H(32)	9534(4)	3775(4)	8883(3)	65

[MnTClPP][TCNE]·$2CH_2Cl_2$

Table 4b. Crystal data and structure refinement for 2.

Identification code	shelxs
Empirical formula	C52 H28 Cl8 Mn N8
Formula weight	1103.36
Temperature	193(2) K
Wavelength	0.71073 A
Crystal system	Monoclinic
Space group	P 21/n
Unit cell dimensions	a = 9.894(2) A alpha = 90 deg. b = 10.697(2) A beta = 101.34(2) deg. c = 23.560(5) A gamma = 90 deg.
Volume	2444.6(8) A^3
Z	2
Density (calculated)	1.499 Mg/m^3
Absorption coefficient	0.754 mm^-1
F(000)	1114
Crystal size	0.38 x 0.26 x 0.25 mm
Theta range for data collection	2.10 to 24.97 deg.
Index ranges	0<=h<=11, 0<=k<=12, -27<=l<=27
Reflections collected	4561
Independent reflections	4294 [R(int) = 0.0148]
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.995 and 0.991
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4284 / 0 / 313
Goodness-of-fit on F^2	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0411, wR2 = 0.1034
R indices (all data)	R1 = 0.0599, wR2 = 0.1196

Largest diff. peak and hole	0.457 and -0.528 e.A^-3

[MnTClPP][TCNE]·2CH_2Cl_2

S7

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for 2. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mn	10000	0	10000	19(1)
Cl(1)	6047(1)	7520(1)	10978(1)	59(1)
Cl(2)	7813(1)	1920(1)	6005(1)	48(1)
Cl(3)	10406(1)	5897(1)	7280(1)	84(1)
Cl(4)	12844(2)	4496(2)	7804(1)	126(1)
N(1)	12125(2)	822(2)	10005(1)	28(1)
N(2)	16142(3)	1001(3)	11183(1)	48(1)
N(3)	9844(2)	903(2)	10732(1)	21(1)
N(4)	9064(2)	1434(2)	9524(1)	21(1)
C(1)	13280(3)	588(3)	10101(1)	26(1)
C(2)	14697(3)	311(3)	10211(1)	27(1)
C(3)	15492(3)	683(3)	10747(1)	31(1)
C(4)	9240(3)	2051(2)	10774(1)	24(1)
C(5)	10708(3)	-2360(3)	8635(1)	30(1)
C(6)	10089(3)	-1402(3)	8312(1)	30(1)
C(7)	9740(3)	-488(3)	8705(1)	24(1)
C(8)	9099(3)	653(3)	8542(1)	23(1)
C(9)	8754(3)	1517(3)	8929(1)	24(1)
C(10)	8000(3)	2647(3)	8763(1)	29(1)
C(11)	7861(3)	3239(3)	9254(1)	29(1)
C(12)	8529(3)	2491(2)	9731(1)	23(1)
C(13)	8613(3)	2794(2)	10310(1)	24(1)
C(14)	7967(3)	3995(2)	10452(1)	26(1)
C(15)	8708(3)	5095(3)	10531(2)	40(1)
C(16)	8118(4)	6192(3)	10678(2)	45(1)
C(17)	6786(4)	6169(3)	10759(1)	37(1)
C(18)	6028(4)	5093(3)	10683(2)	49(1)
C(19)	6618(3)	4008(3)	10526(2)	43(1)
C(20)	8772(3)	967(3)	7908(1)	25(1)
C(21)	7768(3)	320(3)	7529(1)	30(1)
C(22)	7463(3)	623(3)	6945(1)	33(1)
C(23)	8187(3)	1560(3)	6741(1)	32(1)
C(24)	9197(3)	2230(3)	7106(1)	34(1)
C(25)	9473(3)	1930(3)	7691(1)	31(1)
C(26)	12180(4)	5681(5)	7327(2)	69(1)

[MnTClPP][TCNE]·2CH_2Cl_2

Table 55 Bond lengths [A] and angles [deg] for 1.

Mn-N(3)#1	2.009(2)
Mn-N(3)	2.009(2)
Mn-N(4)#1	2.014(2)
Mn-N(4)	2.014(2)
Mn-N(1)	2.276(2)
Mn-N(1)#1	2.276(2)
Cl(1)-C(17)	1.742(3)
Cl(2)-C(23)	1.743(3)
Cl(3)-C(26)	1.752(5)
Cl(4)-C(26)	1.736(5)
N(1)-C(1)	1.148(4)
N(2)-C(3)	1.151(4)
N(3)-C(4)	1.378(3)
N(3)-C(7)#1	1.382(3)
N(4)-C(12)	1.377(3)
N(4)-C(9)	1.379(3)
C(1)-C(2)	1.407(4)
C(2)-C(3)	1.407(4)
C(2)-C(2)#2	1.423(6)
C(4)-C(13)	1.393(4)
C(4)-C(5)#1	1.423(4)
C(5)-C(6)	1.350(4)
C(5)-C(4)#1	1.423(4)
C(6)-C(7)	1.435(4)
C(7)-N(3)#1	1.382(3)
C(7)-C(8)	1.394(4)
C(8)-C(9)	1.387(4)
C(8)-C(20)	1.502(4)
C(9)-C(10)	1.434(4)
C(10)-C(11)	1.349(4)
C(11)-C(12)	1.430(4)
C(12)-C(13)	1.390(4)
C(13)-C(14)	1.501(4)
C(14)-C(15)	1.379(4)
C(14)-C(19)	1.380(4)
C(15)-C(16)	1.385(4)
C(16)-C(17)	1.368(5)
C(17)-C(18)	1.366(5)
C(18)-C(19)	1.382(4)
C(20)-C(21)	1.384(4)
C(20)-C(25)	1.395(4)
C(21)-C(22)	1.389(4)
C(22)-C(23)	1.373(4)
C(23)-C(24)	1.383(4)
C(24)-C(25)	1.389(4)
N(3)#1-Mn-N(3)	180.0
N(3)#1-Mn-N(4)#1	90.42(9)
N(3)-Mn-N(4)#1	89.58(9)
N(3)#1-Mn-N(4)	89.58(9)

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N(3)-Mn-N(4)	90.42(9)
N(4)#1-Mn-N(4)	180.0
N(3)#1-Mn-N(1)	87.90(9)
N(3)-Mn-N(1)	92.10(9)
N(4)#1-Mn-N(1)	88.18(9)
N(4)-Mn-N(1)	91.82(9)
N(3)#1-Mn-N(1)#1	92.10(9)
N(3)-Mn-N(1)#1	87.90(9)
N(4)#1-Mn-N(1)#1	91.82(9)
N(4)-Mn-N(1)#1	88.18(9)
N(1)-Mn-N(1)#1	180.0
C(1)-N(1)-Mn	143.1(2)
C(4)-N(3)-C(7)#1	105.7(2)
C(4)-N(3)-Mn	126.6(2)
C(7)#1-N(3)-Mn	127.6(2)
C(12)-N(4)-C(9)	106.4(2)
C(12)-N(4)-Mn	126.5(2)
C(9)-N(4)-Mn	127.0(2)
N(1)-C(1)-C(2)	179.2(3)
C(3)-C(2)-C(1)	117.9(3)
C(3)-C(2)-C(2)#2	121.4(3)
C(1)-C(2)-C(2)#2	120.7(3)
N(2)-C(3)-C(2)	179.2(3)
N(3)-C(4)-C(13)	125.9(2)
N(3)-C(4)-C(5)#1	110.1(2)
C(13)-C(4)-C(5)#1	124.0(2)
C(6)-C(5)-C(4)#1	107.6(2)
C(5)-C(6)-C(7)	107.1(2)
N(3)#1-C(7)-C(8)	125.4(2)
N(3)#1-C(7)-C(6)	109.7(2)
C(8)-C(7)-C(6)	125.0(2)
C(9)-C(8)-C(7)	124.1(2)
C(9)-C(8)-C(20)	118.1(2)
C(7)-C(8)-C(20)	117.9(2)
N(4)-C(9)-C(8)	126.2(2)
N(4)-C(9)-C(10)	109.3(2)
C(8)-C(9)-C(10)	124.4(2)
C(11)-C(10)-C(9)	107.3(2)
C(10)-C(11)-C(12)	107.6(2)
N(4)-C(12)-C(13)	125.9(2)
N(4)-C(12)-C(11)	109.4(2)
C(13)-C(12)-C(11)	124.7(2)
C(12)-C(13)-C(4)	124.6(2)
C(12)-C(13)-C(14)	118.2(2)
C(4)-C(13)-C(14)	117.2(2)
C(15)-C(14)-C(19)	118.5(3)
C(15)-C(14)-C(13)	121.4(3)
C(19)-C(14)-C(13)	120.1(3)
C(14)-C(15)-C(16)	121.1(3)
C(17)-C(16)-C(15)	119.0(3)
C(18)-C(17)-C(16)	121.0(3)
C(18)-C(17)-Cl(1)	119.1(3)
C(16)-C(17)-Cl(1)	119.9(3)
C(17)-C(18)-C(19)	119.6(3)

C(14)-C(19)-C(18)	120.8(3)
C(21)-C(20)-C(25)	118.6(3)
C(21)-C(20)-C(8)	121.1(2)
C(25)-C(20)-C(8)	120.3(2)
C(20)-C(21)-C(22)	120.8(3)
C(23)-C(22)-C(21)	119.4(3)
C(22)-C(23)-C(24)	121.6(3)
C(22)-C(23)-Cl(2)	119.1(2)
C(24)-C(23)-Cl(2)	119.3(2)
C(23)-C(24)-C(25)	118.3(3)
C(24)-C(25)-C(20)	121.4(3)
Cl(4)-C(26)-Cl(3)	112.6(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y,-z+2 #2 -x+3,-y,-z+2

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Table S4. Anisotropic displacement parameters (A^2 x 10^3) for 2. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Mn	20(1)	17(1)	20(1)	-1(1)	3(1)	4(1)
Cl(1)	93(1)	29(1)	66(1)	4(1)	39(1)	28(1)
Cl(2)	60(1)	56(1)	26(1)	14(1)	4(1)	6(1)
Cl(3)	72(1)	99(1)	92(1)	-38(1)	42(1)	-25(1)
Cl(4)	148(2)	164(2)	67(1)	43(1)	26(1)	11(1)
N(1)	24(1)	28(1)	34(1)	-5(1)	8(1)	0(1)
N(2)	43(2)	63(2)	37(2)	-7(1)	2(1)	3(1)
N(3)	22(1)	21(1)	20(1)	-1(1)	3(1)	4(1)
N(4)	23(1)	19(1)	21(1)	-1(1)	4(1)	4(1)
C(1)	29(2)	22(1)	28(2)	-2(1)	8(1)	-1(1)
C(2)	22(1)	27(2)	32(2)	3(1)	5(1)	3(1)
C(3)	27(2)	33(2)	35(2)	2(1)	10(1)	6(1)
C(4)	24(1)	20(1)	27(1)	-3(1)	5(1)	4(1)
C(5)	36(2)	27(2)	27(2)	-3(1)	7(1)	8(1)
C(6)	35(2)	30(2)	25(1)	-3(1)	6(1)	7(1)
C(7)	24(1)	24(1)	22(1)	-2(1)	4(1)	0(1)
C(8)	23(1)	24(1)	22(1)	0(1)	3(1)	1(1)
C(9)	24(1)	22(1)	25(1)	3(1)	3(1)	1(1)
C(10)	34(2)	26(2)	28(2)	4(1)	4(1)	9(1)
C(11)	32(2)	22(1)	34(2)	3(1)	5(1)	11(1)
C(12)	22(1)	19(1)	28(1)	1(1)	5(1)	4(1)
C(13)	24(1)	19(1)	29(2)	-1(1)	6(1)	4(1)
C(14)	32(2)	21(1)	24(1)	0(1)	5(1)	7(1)
C(15)	42(2)	30(2)	53(2)	-7(2)	23(2)	1(1)
C(16)	63(2)	22(2)	58(2)	-5(2)	26(2)	-1(2)
C(17)	55(2)	23(2)	34(2)	5(1)	16(2)	17(1)
C(18)	38(2)	39(2)	74(3)	-3(2)	21(2)	11(2)
C(19)	35(2)	27(2)	69(2)	-7(2)	13(2)	3(1)
C(20)	28(1)	24(1)	24(1)	1(1)	5(1)	7(1)
C(21)	35(2)	25(1)	28(1)	4(1)	5(1)	0(1)
C(22)	38(2)	31(2)	26(2)	-1(1)	1(1)	1(1)
C(23)	40(2)	31(2)	23(1)	5(1)	6(1)	11(1)
C(24)	39(2)	30(2)	35(2)	6(1)	9(1)	0(1)
C(25)	33(2)	29(2)	30(2)	0(1)	4(1)	-2(1)
C(26)	64(3)	89(3)	59(3)	-5(2)	21(2)	-25(2)

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Table S1D. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for 2.

	x	y	z	U(eq)
H(5)	11048(3)	-3104(3)	8493(1)	36
H(6)	9917(3)	-1344(3)	7902(1)	36
H(10)	7660(3)	2927(3)	8379(1)	35
H(11)	7404(3)	4012(3)	9279(1)	35
H(15)	9639(3)	5100(3)	10483(2)	48
H(16)	8630(4)	6949(3)	10722(2)	55
H(18)	5102(4)	5091(3)	10737(2)	59
H(19)	6088(3)	3261(3)	10468(2)	52
H(21)	7282(3)	-339(3)	7671(1)	35
H(22)	6759(3)	186(3)	6689(1)	39
H(24)	9690(3)	2879(3)	6960(1)	41
H(25)	10154(3)	2391(3)	7948(1)	37
H(26A)	12356(4)	5479(5)	6938(2)	83
H(26B)	12666(4)	6472(5)	7455(2)	83