Supporting Information

Synthesis of 2: MeLi (1.5 mL, 1.6 M in diethyl ether, 2.4 mmol) was added to a suspension of **1** (1.20 g, 1 mmol) in toluene (40 mL) at –78 °C. The mixture was allowed to warm to room temperature and stirred for 14 h. All the volatiles were removed in vacuum and the residue was extracted with hexane (2×15 mL). The yellow solution was concentrated to ca. 15 mL and kept at room temperature for 24 h to give yellow crystals. The crystals were collected by filtration and the filtrate was concentrated and kept at 4 °C for one week to give additional crystals of **2**. Total yield: 0.51 g (52%). Mp: 190-192 °C. Anal. Calcd for $C_{60}H_{88}Mn_2N_4$ (975.22): C, 73.83; H, 9.02; N, 5.74. Found: C, 73.31; H, 8.76; N, 5.64. EI–MS: *m/z* (%) 487 (6) $[LMnMe]^+$, 472 (100) $[LMn]^+$. IR (KBr, Nujol mull, cm^{-1}): $\tilde{\nu}$ 1658 (w), 1624 (w), 1589 (w), 1552 (w), 1525 (w), 1314 (w), 1261 (m), 1174 (w), 1098 (w), 1040 (w), 1021 (w), 936 (w), 798 (m), 759 (w), 721 (w), 662 (w), 563 (w).

Synthesis of 3: The precedure is the same as that described for **2**. Yield: 65%. Mp: 230-232 °C. Anal. Calcd for $C_{35}H_{46}MnN_2$ (549.68): C, 76.41; H, 8.37; N, 5.09. Found: C, 75.72; H, 8.13; N, 4.86. EI–MS: *m/z* (%) 549 (3) $[M]^+$, 471 (100) $[M\text{-}C_6H_6]^+$. IR (KBr, Nujol mull, cm^{-1}): $\tilde{\nu}$ 1660 (w), 1640 (w), 1625 (w), 1590 (w), 1553 (w), 1531 (w), 1312 (w), 1261 (m), 1170 (w), 1095 (m), 1021 (m), 937 (w), 873 (w), 799 (m), 761 (w), 724 (w), 674 (w), 643 (w), 613 (w), 604 (w), 583 (w), 525 (w), 463 (w).

Table 1. Crystal data and structure refinement for **2**.

Empirical formula	C30 H44 Mn N2
Formula weight	487.61
Temperature	133(2) K
Wavelength	0.71073 A
Crystal system, space group	monoclinic, C 2/c
Unit cell dimensions	a = 22.612(5) A alpha = 90 deg. b = 14.880(3) A beta = 90.05(3) deg. c = 16.481(3) A gamma = 90 deg.
Volume	5545.2(19) A^3
Z, Calculated density	8, 1.168 Mg/m^3
Absorption coefficient	0.495 mm^-1
F(000)	2104
Theta range for data collection	1.64 to 24.71 deg.
Index ranges	-26<=h<=26, -17<=k<=17, -19<=l<=19
Reflections collected / unique	20857 / 4662 [R(int) = 0.0360]
Observed reflections [I>2sigma(I)]	4032
Completeness to theta = 24.71	98.8%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4662 / 0 / 320
Goodness-of-fit on F^2	1.068
Final R indices [I>2sigma(I)]	R1 = 0.0327, wR2 = 0.0736
R indices (all data)	R1 = 0.0413, wR2 = 0.0772
Largest diff. peak and hole	0.257 and -0.260 e.A^-3

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

	x	y	z	U(eq)
Mn(1)	0.7041(1)	0.8135(1)	0.5024(1)	0.01703(9)
N(1)	0.6960(1)	0.9483(1)	0.5436(1)	0.0188(3)
N(2)	0.6160(1)	0.8191(1)	0.4570(1)	0.0188(3)
C(1)	0.6593(1)	1.1049(1)	0.5324(1)	0.0288(5)
C(2)	0.6572(1)	1.0058(1)	0.5114(1)	0.0203(4)
C(3)	0.6113(1)	0.9815(1)	0.4588(1)	0.0219(4)
C(4)	0.5890(1)	0.8963(1)	0.4394(1)	0.0203(4)
C(5)	0.5290(1)	0.8974(1)	0.3977(1)	0.0285(4)
C(6)	0.7322(1)	0.9833(1)	0.6082(1)	0.0214(4)
C(7)	0.7136(1)	0.9695(1)	0.6888(1)	0.0257(4)
C(8)	0.7461(1)	1.0091(2)	0.7509(1)	0.0348(5)
C(9)	0.7968(1)	1.0581(2)	0.7344(1)	0.0393(5)
C(10)	0.8157(1)	1.0682(1)	0.6558(1)	0.0342(5)
C(11)	0.7840(1)	1.0326(1)	0.5908(1)	0.0251(4)
C(12)	0.6576(1)	0.9163(1)	0.7079(1)	0.0293(4)
C(13)	0.6634(1)	0.8563(2)	0.7823(1)	0.0407(5)
C(14)	0.6045(1)	0.9796(2)	0.7171(2)	0.0424(6)
C(15)	0.8048(1)	1.0487(1)	0.5043(1)	0.0271(4)
C(16)	0.8591(1)	0.9912(2)	0.4860(2)	0.0399(5)
C(17)	0.8194(1)	1.1475(2)	0.4871(2)	0.0476(6)
C(18)	0.5824(1)	0.7387(1)	0.4405(1)	0.0197(4)
C(19)	0.5473(1)	0.7020(1)	0.5028(1)	0.0224(4)
C(20)	0.5114(1)	0.6285(1)	0.4842(1)	0.0270(4)
C(21)	0.5117(1)	0.5906(1)	0.4078(1)	0.0294(5)
C(22)	0.5483(1)	0.6249(1)	0.3481(1)	0.0273(4)
C(23)	0.5836(1)	0.7002(1)	0.3627(1)	0.0229(4)
C(24)	0.5463(1)	0.7422(1)	0.5876(1)	0.0277(4)
C(25)	0.4922(1)	0.8014(2)	0.6004(2)	0.0517(7)
C(26)	0.5498(1)	0.6712(2)	0.6542(1)	0.0395(5)
C(27)	0.6209(1)	0.7391(1)	0.2943(1)	0.0256(4)
C(28)	0.5844(1)	0.7647(2)	0.2198(1)	0.0400(5)
C(29)	0.6686(1)	0.6728(2)	0.2688(2)	0.0505(7)
C(30)	0.7243(1)	0.7077(2)	0.5952(1)	0.0247(4)

Table 3. Bond lengths [pm] and angles [deg] for **2**.

Mn(1)-N(1)	212.5(2)
Mn(1)-N(2)	212.9(2)
Mn(1)-C(30)	224.1(2)
Mn(1)-C(30)#1	230.6(2)
Mn(1)-Mn(1)#1	280.9(1)
N(1)-C(2)	133.5(2)
N(1)-C(6)	143.9(2)
N(2)-C(4)	133.3(2)
N(2)-C(18)	144.3(2)
C(1)-C(2)	151.6(3)
C(2)-C(3)	139.9(3)
C(3)-C(4)	140.2(3)
C(4)-C(5)	151.9(3)
C(6)-C(7)	140.9(3)
C(6)-C(11)	141.2(3)
C(7)-C(8)	139.0(3)
C(7)-C(12)	152.5(3)
C(8)-C(9)	138.7(3)
C(9)-C(10)	137.4(3)
C(10)-C(11)	139.2(3)
C(11)-C(15)	152.2(3)
C(12)-C(13)	152.3(3)
C(12)-C(14)	153.5(3)
C(15)-C(16)	152.6(3)
C(15)-C(17)	153.4(3)
C(18)-C(23)	140.6(3)
C(18)-C(19)	140.8(3)
C(19)-C(20)	139.6(3)
C(19)-C(24)	152.1(3)
C(20)-C(21)	137.9(3)
C(21)-C(22)	138.3(3)
C(22)-C(23)	139.7(3)
C(23)-C(27)	152.3(3)
C(24)-C(25)	152.4(3)
C(24)-C(26)	152.5(3)
C(27)-C(29)	152.1(3)
C(27)-C(28)	152.7(3)
N(1)-Mn(1)-N(2)	89.68(6)
N(1)-Mn(1)-C(30)	117.53(8)
N(2)-Mn(1)-C(30)	117.18(8)
N(1)-Mn(1)-C(30)#1	114.41(7)
N(2)-Mn(1)-C(30)#1	114.72(8)
C(30)-Mn(1)-C(30)#1	103.71(7)
N(1)-Mn(1)-Mn(1)#1	135.07(4)
N(2)-Mn(1)-Mn(1)#1	135.05(4)
C(30)-Mn(1)-Mn(1)#1	52.89(6)
C(30)#1-Mn(1)-Mn(1)#1	50.82(5)
C(2)-N(1)-C(6)	115.77(15)
C(2)-N(1)-Mn(1)	122.29(12)
C(6)-N(1)-Mn(1)	121.93(11)
C(4)-N(2)-C(18)	115.59(15)
C(4)-N(2)-Mn(1)	122.61(12)
C(18)-N(2)-Mn(1)	121.76(11)
N(1)-C(2)-C(3)	124.60(16)
N(1)-C(2)-C(1)	120.83(17)
C(3)-C(2)-C(1)	114.55(16)
C(2)-C(3)-C(4)	129.93(17)
N(2)-C(4)-C(3)	124.36(17)
N(2)-C(4)-C(5)	121.11(16)

C(3)-C(4)-C(5)	114.50(16)
C(7)-C(6)-C(11)	121.01(18)
C(7)-C(6)-N(1)	118.35(16)
C(11)-C(6)-N(1)	120.61(17)
C(8)-C(7)-C(6)	118.33(19)
C(8)-C(7)-C(12)	120.44(18)
C(6)-C(7)-C(12)	121.17(18)
C(9)-C(8)-C(7)	121.0(2)
C(10)-C(9)-C(8)	120.0(2)
C(9)-C(10)-C(11)	121.6(2)
C(10)-C(11)-C(6)	117.96(19)
C(10)-C(11)-C(15)	120.08(18)
C(6)-C(11)-C(15)	121.95(18)
C(13)-C(12)-C(7)	113.53(18)
C(13)-C(12)-C(14)	110.29(17)
C(7)-C(12)-C(14)	110.57(18)
C(11)-C(15)-C(16)	110.30(17)
C(11)-C(15)-C(17)	112.92(18)
C(16)-C(15)-C(17)	109.22(18)
C(23)-C(18)-C(19)	121.21(17)
C(23)-C(18)-N(2)	119.96(16)
C(19)-C(18)-N(2)	118.80(16)
C(20)-C(19)-C(18)	118.20(18)
C(20)-C(19)-C(24)	120.06(17)
C(18)-C(19)-C(24)	121.70(16)
C(21)-C(20)-C(19)	121.12(18)
C(20)-C(21)-C(22)	120.13(18)
C(21)-C(22)-C(23)	121.05(19)
C(22)-C(23)-C(18)	118.19(17)
C(22)-C(23)-C(27)	119.65(17)
C(18)-C(23)-C(27)	122.14(16)
C(19)-C(24)-C(25)	111.57(18)
C(19)-C(24)-C(26)	112.87(17)
C(25)-C(24)-C(26)	109.95(17)
C(29)-C(27)-C(23)	110.54(17)
C(29)-C(27)-C(28)	108.84(18)
C(23)-C(27)-C(28)	112.93(16)

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

Table 4. Anisotropic displacement parameters (A^2) 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(1)	0.01586(14)	0.01546(14)	0.01975(14)	-0.00048(11)	-0.00027(10)	0.00121(11)
N(1)	0.0172(7)	0.0184(8)	0.0209(8)	-0.0022(6)	-0.0003(6)	0.0010(6)
N(2)	0.0175(7)	0.0176(7)	0.0212(8)	-0.0002(6)	-0.0014(6)	-0.0013(6)
C(1)	0.0315(11)	0.0186(10)	0.0365(12)	-0.0038(8)	-0.0024(9)	0.0034(8)
C(2)	0.0216(9)	0.0165(9)	0.0228(9)	-0.0001(7)	0.0046(7)	0.0011(7)
C(3)	0.0220(9)	0.0172(9)	0.0264(10)	0.0031(8)	-0.0015(8)	0.0037(7)
C(4)	0.0182(9)	0.0224(9)	0.0205(9)	0.0011(7)	0.0004(7)	0.0016(7)
C(5)	0.0241(10)	0.0250(10)	0.0363(12)	0.0045(8)	-0.0075(9)	0.0010(8)
C(6)	0.0228(9)	0.0169(9)	0.0246(10)	-0.0053(8)	-0.0024(8)	0.0039(7)
C(7)	0.0271(10)	0.0241(10)	0.0259(10)	-0.0061(8)	0.0005(8)	0.0035(8)
C(8)	0.0382(12)	0.0403(12)	0.0260(11)	-0.0123(9)	-0.0004(9)	0.0032(10)
C(9)	0.0370(12)	0.0427(13)	0.0382(13)	-0.0202(10)	-0.0110(10)	-0.0009(10)
C(10)	0.0290(11)	0.0298(11)	0.0439(13)	-0.0109(10)	-0.0052(10)	-0.0046(9)
C(11)	0.0222(9)	0.0194(9)	0.0336(11)	-0.0030(8)	-0.0024(8)	0.0022(7)
C(12)	0.0295(10)	0.0342(11)	0.0242(10)	-0.0042(9)	0.0040(8)	0.0004(9)
C(13)	0.0410(13)	0.0456(13)	0.0354(12)	0.0060(10)	0.0101(10)	0.0056(10)
C(14)	0.0302(12)	0.0520(15)	0.0451(14)	0.0055(11)	0.0071(10)	0.0056(10)
C(15)	0.0232(10)	0.0230(10)	0.0351(11)	0.0032(8)	-0.0016(9)	-0.0019(8)
C(16)	0.0320(12)	0.0419(13)	0.0459(14)	0.0035(11)	0.0084(11)	0.0060(10)
C(17)	0.0499(14)	0.0309(12)	0.0620(17)	0.0111(11)	0.0050(13)	-0.0043(11)
C(18)	0.0148(8)	0.0168(9)	0.0276(10)	0.0018(7)	-0.0034(7)	0.0016(7)
C(19)	0.0178(9)	0.0208(10)	0.0287(10)	0.0033(8)	-0.0011(8)	0.0017(7)
C(20)	0.0208(9)	0.0243(10)	0.0360(11)	0.0082(9)	-0.0017(8)	-0.0027(8)
C(21)	0.0277(10)	0.0191(10)	0.0412(12)	0.0039(9)	-0.0088(9)	-0.0057(8)
C(22)	0.0282(10)	0.0212(10)	0.0325(11)	-0.0019(8)	-0.0104(9)	-0.0001(8)
C(23)	0.0206(9)	0.0211(10)	0.0269(10)	0.0008(8)	-0.0047(8)	0.0019(7)
C(24)	0.0251(10)	0.0285(10)	0.0296(11)	0.0020(8)	0.0056(8)	-0.0038(8)
C(25)	0.0607(16)	0.0484(15)	0.0462(14)	-0.0005(12)	0.0085(12)	0.0249(13)
C(26)	0.0444(13)	0.0445(14)	0.0296(11)	0.0038(10)	0.0055(10)	0.0090(10)
C(27)	0.0250(10)	0.0267(10)	0.0251(10)	-0.0022(8)	-0.0018(8)	-0.0029(8)
C(28)	0.0349(12)	0.0489(14)	0.0362(12)	0.0167(11)	-0.0047(10)	-0.0078(10)
C(29)	0.0449(14)	0.0613(17)	0.0451(14)	0.0073(12)	0.0130(12)	0.0193(12)
C(30)	0.0223(11)	0.0222(11)	0.0297(12)	0.0051(9)	0.0024(9)	0.0078(8)

Table 5. Hydrogen coordinates and isotropic displacement parameters (A^2) for **2**.

	x	y	z	U(eq)
H(1A)	0.6716	1.1122	0.5890	0.043
H(1B)	0.6200	1.1314	0.5248	0.043
H(1C)	0.6876	1.1354	0.4968	0.043
H(3A)	0.5925	1.0303	0.4320	0.026
H(5A)	0.5054	0.8465	0.4169	0.043
H(5B)	0.5345	0.8927	0.3389	0.043
H(5C)	0.5086	0.9537	0.4105	0.043
H(8A)	0.7333	1.0024	0.8055	0.042
H(9A)	0.8185	1.0847	0.7776	0.047

H(10A)	0.8513	1.1002	0.6454	0.041
H(12A)	0.6495	0.8764	0.6603	0.035
H(13A)	0.6278	0.8193	0.7878	0.061
H(13B)	0.6682	0.8937	0.8308	0.061
H(13C)	0.6980	0.8172	0.7762	0.061
H(14A)	0.5988	1.0133	0.6666	0.064
H(14B)	0.6119	1.0216	0.7618	0.064
H(14C)	0.5689	0.9443	0.7288	0.064
H(15A)	0.7724	1.0299	0.4666	0.033
H(16A)	0.8699	0.9979	0.4287	0.060
H(16B)	0.8501	0.9280	0.4973	0.060
H(16C)	0.8922	1.0107	0.5201	0.060
H(17A)	0.8273	1.1554	0.4291	0.071
H(17B)	0.8543	1.1652	0.5185	0.071
H(17C)	0.7857	1.1852	0.5029	0.071
H(20A)	0.4862	0.6042	0.5248	0.032
H(21A)	0.4867	0.5409	0.3961	0.035
H(22A)	0.5493	0.5968	0.2963	0.033
H(24A)	0.5820	0.7814	0.5930	0.033
H(25A)	0.4930	0.8265	0.6554	0.078
H(25B)	0.4562	0.7654	0.5934	0.078
H(25C)	0.4924	0.8505	0.5608	0.078
H(26A)	0.5545	0.7008	0.7070	0.059
H(26B)	0.5837	0.6318	0.6442	0.059
H(26C)	0.5134	0.6355	0.6543	0.059
H(27A)	0.6408	0.7946	0.3149	0.031
H(28A)	0.6102	0.7921	0.1790	0.060
H(28B)	0.5536	0.8077	0.2356	0.060
H(28C)	0.5658	0.7107	0.1972	0.060
H(29A)	0.6951	0.7016	0.2295	0.076
H(29B)	0.6501	0.6201	0.2438	0.076
H(29C)	0.6913	0.6541	0.3165	0.076
H(30C)	0.7426(15)	0.663(2)	0.608(2)	0.077(11)
H(30B)	0.6920(18)	0.693(2)	0.595(2)	0.085(12)
H(30A)	0.7296(17)	0.736(3)	0.632(2)	0.092(14)

Table 6. Crystal data and structure refinement for **3**.

Empirical formula	C35 H46 Mn N2
Formula weight	549.68
Temperature	133(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, P nma
Unit cell dimensions	a = 16.6103(13) A alpha = 90 deg. b = 20.943(2) A beta = 90 deg. c = 9.2785(13) A gamma = 90 deg.
Volume	3227.8(6) A^3
Z, Calculated density	4, 1.131 Mg/m^3
Absorption coefficient	0.433 mm^-1
F(000)	1180
Theta range for data collection	1.94 to 22.99 deg.
Index ranges	-16<=h<=16, -23<=k<=22, -8<=l<=10
Reflections collected / unique	8044 / 2191 [R(int) = 0.0751]
Observed reflections [I>2sigma(I)]	1604
Completeness to theta = 22.99	94.5%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2191 / 0 / 183
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0514, wR2 = 0.1188
R indices (all data)	R1 = 0.0758, wR2 = 0.1296
Largest diff. peak and hole	0.199 and -0.408 e.A^-3

Table 7. Atomic coordinates and equivalent isotropic displacement parameters (A^2) for **3**.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Mn(1)	0.3875(1)	0.2500	0.1102(1)	0.0388(3)
N(1)	0.3234(2)	0.3197(1)	0.2125(3)	0.0362(7)
C(1)	0.2215(2)	0.3675(1)	0.3717(4)	0.0450(10)
C(2)	0.2609(2)	0.3103(1)	0.3004(4)	0.0382(9)
C(3)	0.2298(3)	0.2500	0.3362(6)	0.0394(13)
C(4)	0.3579(2)	0.3828(1)	0.1941(4)	0.0366(9)
C(5)	0.3288(2)	0.4223(2)	0.0835(4)	0.0408(10)
C(6)	0.3686(3)	0.4808(2)	0.0602(5)	0.0486(11)
C(7)	0.4332(3)	0.4986(2)	0.1434(5)	0.0493(11)
C(8)	0.4609(2)	0.4588(2)	0.2504(5)	0.0482(10)
C(9)	0.4233(2)	0.4005(2)	0.2789(4)	0.0410(9)
C(10)	0.2599(2)	0.4025(2)	-0.0142(4)	0.0445(10)
C(11)	0.2928(3)	0.3788(2)	-0.1591(5)	0.0738(14)
C(12)	0.1975(3)	0.4549(2)	-0.0379(6)	0.0661(13)
C(13)	0.4557(3)	0.3582(2)	0.3996(5)	0.0527(11)
C(14)	0.5424(3)	0.3378(2)	0.3710(5)	0.0656(13)
C(15)	0.4502(3)	0.3925(3)	0.5456(5)	0.0759(15)
C(16)	0.4849(3)	0.2500	-0.0302(6)	0.0401(13)
C(17)	0.5201(2)	0.3069(2)	-0.0817(4)	0.0465(10)
C(18)	0.5845(3)	0.3071(2)	-0.1772(4)	0.0510(11)
C(19)	0.6170(4)	0.2500	-0.2265(6)	0.0527(15)

Table 8. Bond lengths [pm] and angles [deg] for **3**.

Mn(1)-N(1)	204.1(3)
Mn(1)-N(1)#1	204.1(3)
Mn(1)-C(16)	207.7(6)
N(1)-C(2)	133.5(5)
N(1)-C(4)	145.0(4)
C(1)-C(2)	151.6(5)
C(2)-C(3)	140.5(4)
C(3)-C(2)#1	140.5(4)
C(4)-C(9)	139.2(5)
C(4)-C(5)	140.4(5)
C(5)-C(6)	140.8(5)
C(5)-C(10)	151.8(6)
C(6)-C(7)	137.3(6)
C(7)-C(8)	137.6(6)
C(8)-C(9)	139.7(5)
C(9)-C(13)	152.6(5)
C(10)-C(12)	152.6(5)
C(10)-C(11)	153.3(6)
C(13)-C(14)	152.5(6)
C(13)-C(15)	153.6(6)
C(16)-C(17)#1	141.2(5)
C(16)-C(17)	141.2(5)
C(17)-C(18)	138.8(6)
C(18)-C(19)	139.0(5)
C(19)-C(18)#1	139.0(5)
N(1)-Mn(1)-N(1)#1	91.31(16)
N(1)-Mn(1)-C(16)	134.27(8)
N(1)#1-Mn(1)-C(16)	134.28(8)
C(2)-N(1)-C(4)	120.8(3)
C(2)-N(1)-Mn(1)	125.8(2)
C(4)-N(1)-Mn(1)	113.0(2)
N(1)-C(2)-C(3)	124.2(3)
N(1)-C(2)-C(1)	119.1(3)
C(3)-C(2)-C(1)	116.6(4)
C(2)#1-C(3)-C(2)	128.1(5)
C(9)-C(4)-C(5)	121.7(3)
C(9)-C(4)-N(1)	118.9(3)
C(5)-C(4)-N(1)	119.2(3)
C(4)-C(5)-C(6)	117.6(4)
C(4)-C(5)-C(10)	122.3(3)
C(6)-C(5)-C(10)	120.0(3)
C(7)-C(6)-C(5)	121.1(4)
C(6)-C(7)-C(8)	120.2(3)
C(7)-C(8)-C(9)	121.1(4)
C(4)-C(9)-C(8)	118.3(4)
C(4)-C(9)-C(13)	122.4(3)
C(8)-C(9)-C(13)	119.3(4)
C(5)-C(10)-C(12)	113.7(3)
C(5)-C(10)-C(11)	110.1(4)
C(12)-C(10)-C(11)	110.4(4)
C(9)-C(13)-C(14)	111.6(4)
C(9)-C(13)-C(15)	110.8(3)
C(14)-C(13)-C(15)	109.9(4)
C(17)#1-C(16)-C(17)	115.3(5)
C(17)#1-C(16)-Mn(1)	122.3(3)
C(17)-C(16)-Mn(1)	122.3(3)
C(18)-C(17)-C(16)	122.5(4)
C(17)-C(18)-C(19)	120.5(4)
C(18)-C(19)-C(18)#1	118.7(6)

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

Table 9. Anisotropic displacement parameters (A^2) for 3.
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(1)	0.0393(5)	0.0219(4)	0.0552(5)	0.000	0.0080(4)	0.000
N(1)	0.038(2)	0.0198(13)	0.051(2)	0.0036(12)	0.0017(15)	-0.0018(12)
C(1)	0.047(3)	0.0243(17)	0.064(3)	-0.0026(16)	0.008(2)	0.0020(15)
C(2)	0.037(3)	0.0247(17)	0.053(2)	0.0006(15)	0.0013(18)	0.0013(15)
C(3)	0.037(4)	0.029(2)	0.052(3)	0.000	0.010(2)	0.000
C(4)	0.036(2)	0.0199(16)	0.054(2)	-0.0003(15)	0.0070(17)	-0.0012(14)
C(5)	0.043(3)	0.0254(17)	0.054(3)	-0.0001(16)	0.0052(18)	0.0029(14)
C(6)	0.053(3)	0.0275(18)	0.065(3)	0.0097(17)	0.011(2)	0.0005(16)
C(7)	0.051(3)	0.0252(18)	0.072(3)	-0.0021(18)	0.013(2)	-0.0079(17)
C(8)	0.048(3)	0.0323(19)	0.065(3)	-0.0098(18)	0.007(2)	-0.0075(17)
C(9)	0.040(2)	0.0296(18)	0.054(2)	-0.0041(16)	0.0069(19)	-0.0036(16)
C(10)	0.041(3)	0.0352(19)	0.058(3)	0.0078(17)	-0.0003(19)	0.0007(16)
C(11)	0.059(4)	0.093(3)	0.069(3)	-0.010(3)	-0.005(2)	-0.004(3)
C(12)	0.050(3)	0.043(2)	0.105(4)	0.019(2)	-0.006(3)	0.0040(19)
C(13)	0.051(3)	0.039(2)	0.068(3)	0.0008(19)	-0.008(2)	-0.0064(17)
C(14)	0.063(3)	0.057(3)	0.076(3)	-0.008(2)	-0.004(3)	0.016(2)
C(15)	0.073(4)	0.095(4)	0.059(3)	0.001(3)	0.000(3)	0.020(3)
C(16)	0.039(4)	0.028(2)	0.054(3)	0.000	-0.003(3)	0.000
C(17)	0.039(3)	0.0341(19)	0.066(3)	0.0054(18)	0.004(2)	0.0008(16)
C(18)	0.040(3)	0.048(2)	0.066(3)	0.014(2)	0.002(2)	-0.0045(18)
C(19)	0.041(4)	0.063(4)	0.055(4)	0.000	0.005(3)	0.000

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

	x	y	z	U(eq)
H(1A)	0.2085	0.3996	0.2984	0.067
H(1B)	0.2585	0.3860	0.4425	0.067
H(1C)	0.1720	0.3539	0.4202	0.067
H(3A)	0.1817	0.2500	0.3915	0.047
H(6A)	0.3505	0.5084	-0.0144	0.058
H(7A)	0.4587	0.5385	0.1271	0.059
H(8A)	0.5064	0.4712	0.3058	0.058
H(10A)	0.2319	0.3657	0.0329	0.053
H(11A)	0.3312	0.3441	-0.1424	0.111
H(11B)	0.3199	0.4140	-0.2089	0.111
H(11C)	0.2482	0.3632	-0.2187	0.111
H(12A)	0.1792	0.4712	0.0555	0.099
H(12B)	0.1515	0.4374	-0.0910	0.099
H(12C)	0.2217	0.4898	-0.0936	0.099
H(13A)	0.4216	0.3189	0.4044	0.063
H(14A)	0.5613	0.3109	0.4505	0.098
H(14B)	0.5767	0.3757	0.3635	0.098
H(14C)	0.5449	0.3136	0.2806	0.098
H(15A)	0.4658	0.3630	0.6226	0.114
H(15B)	0.3949	0.4070	0.5615	0.114
H(15C)	0.4865	0.4293	0.5457	0.114
H(17A)	0.4990	0.3467	-0.0499	0.056
H(18A)	0.6064	0.3465	-0.2090	0.061
H(19A)	0.6607	0.2500	-0.2927	0.063