Electronic Supplementary Material (ESI) for Chemical Communications

Supporting Information for

An isolable, metastable, geometrically unique manganese(IV) trihydrazide complex poised for reactivity.

*Shivaiah Vaddypally, Sandeep Kondaveeti, Michael J. Zdilla**

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General: All manipulations were performed under an anaerobic, dry atmosphere of nitrogen gas using standard Glove Box and Schlenk line techniques. All reagents were used as purchased from commercial sources (Aldrich or Strem Chemical) unless otherwise noted. Solvents were distilled from sodium benzophenone ketyl (THF, Et_2O, HMDS), or purified using an Innovative Technology PurSolv solvent purification system (all other solvents) and stored in the glove box over activated 4 Å molecular sieves for 24 h before use. MnF_3, $MnCl_2$, $Mn(OAc)_3$ were purchased from Strem chemicals. Li^{t}BuNH is synthesized according to literature procedure.[4] $Mn[N(SiMe_3)_2]_2$ was prepared from the literature protocol.[5] Benzene-d_6 was stored over 4 Å molecular sieves or Na/Pb alloy[14] for 24 h prior to use. X-Ray structural determinations were performed on a Bruker APEX II DUO diffractometer equipped with an Oxford Cryosystems Cryostream low temperature device. ^{1}H NMR spectra were recorded in benzene-d_6 on a Bruker Advance 400 MHz spectrometer. UV-visible spectra were recorded on UV-1800 Shimadzu UV spectrophotometer. GC-MS analyses were performed on Hewlett Packard, HP 6890 GC system. FT-IR spectra were recorded in the range of 400-4000 cm1-on a Nicolet Varian Cary 380 FT-IR under nitrogen atmosphere using a KBr pellet press. Elemental analyses were carried out by Midwest Microlab, LLC, Indianapolis, IN.

General procedure for Preparation of $Li_2Mn(IV)(dph)_3L_2$ (L = THF, Et_2O; dph = *N,N'*-diphenylhydrazide). 0.1 mmol of Mn precursor was suspended/dissolved in 10 mL dry THF followed by addition 0.047 g (0.6 mmol) LiNH^{t}Bu and stirred for 20 minutes. To this mixture, 0.4 mmol of hydrazide source (diphenyl hydrazine or azobenzene) was added. The resulting green mixture is stirred an additional 15 minutes and filtered. The filtrate is concentrated under vacuum to ca. 2 ml, and crystallized at room temperature by vapor diffusion of *n*-pentane or hexamethyldisiloxane as precipitant. The dark brown crystals are filtered after 24 hrs and dried in vacuo.

$Li_2Mn(IV)(dph)_3(Et_2O)_2$ (**1a**) was prepared by the general procedure with the following changes: The reaction mixture is dried and extracted into diethyl ether, and filtered. The resulting blue filtrate is concentrated and crystallized by slow evaporation of the ether solution of 1a hexamethyldisiloxane in a vapor diffusion double vial setup. This procedure results in formation of dark brown crystals, which are further washed with pentane to remove azobenzene. Yields based on Mn are given in Table 2. UV-Vis (C_6H_6): λ_{max}[nm] (log ε, assignment) = 280 (3.33, ct), 380 (2.44, ct), 631 (2.40, *d*-*d*)., Anal. Calcd for $C_{44}H_{50}Li_2MnN_6O_2$: C, 69.19; H, 6.60; N, 11.00. Found: C, 68.90; H, 5.81; N, 10.58.

$Li_2Mn(IV)(dph)_3(THF)_2$ (1b) was prepared by the general procedure using 0 .037 g (0.1 mmol) of $Mn(NR_2)_2$, 10 mL dry THF, 0.047 g LiNH^{t}Bu (0.6mmol) and 0.0736 g (0.4 mmol) of diphenlydrazine. Yield. 0.062 g (0.082 mmol, 82% based on Mn). ^{1}H NMR (400 MHz, C_6D_6 w/ excess THF): δ = -10.6 (br, 2H, NPh-*p*-H), ,1.3 (v. br., THF), 3.4 (v. br. THF), 6.6 (s, 10 H), 9.7 (br, 4 H, NPh-*o*-H), 10.9 (v. br. 4H, NPh-*m*-H).

Table S1. Synthetic conditions and yields[a] for preparation of **1a** and **1b**.

Mn source	dph^{2-} source[b]	Yield (%)	L[c]
MnF_3	dph	28	Et_2O
$Mn(OAc)_3$	dph	54	Et_2O
$MnCl_2$	dph	61	Et_2O
$Mn[N(SiMe_3)_2]_2$	dph	82	THF
$MnCl_2$	azobenzene	23	Et_2O
$Mn(OAc)_3$	azobenzene	23	Et_2O

[a] Yields are calculated based on Mn. [b] Ligand source is either *N*,*N*'-diphenylhydrazine (dph) or azobenzene. [c] **1a** L = Et_2O, **1b** L = THF.

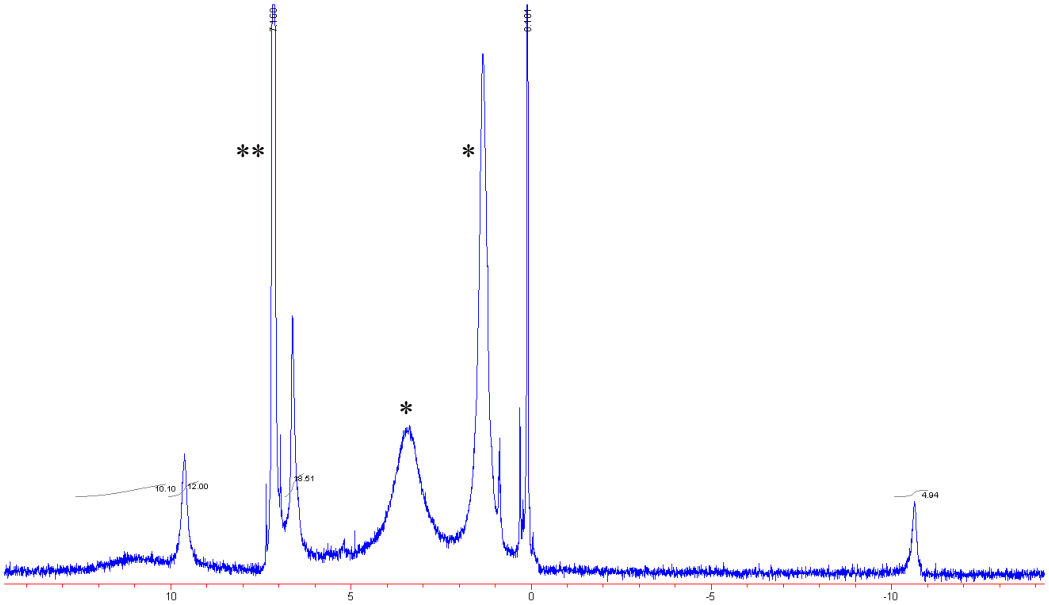

Figure S1. ^{1}H NMR spectrum of **1b** in C_6D_6 with excess THF ligand.* Residual protiosolvent signal indicated by **.

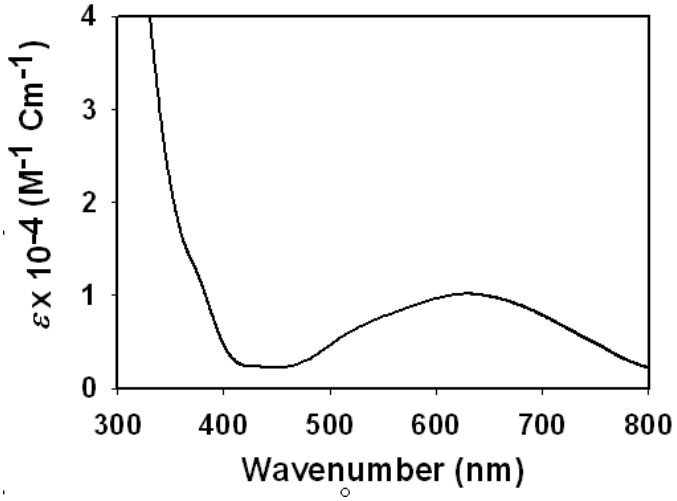

Figure S2. UV-Visible absorption spectrum of **1a** in Benzene.

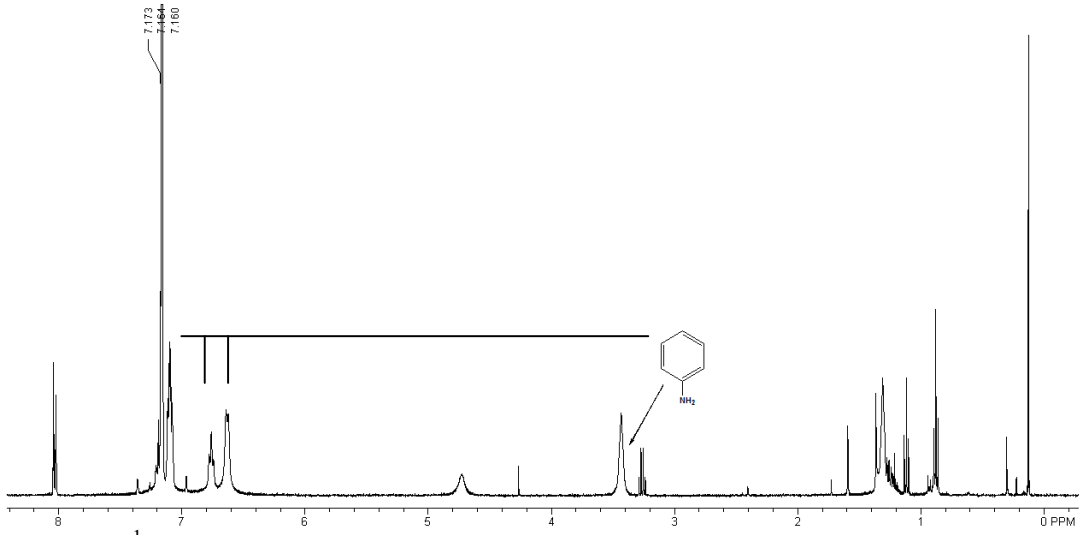

Figure S3. ^{1}H-NMR of pentane filtrate from synthesis of **1** in C_6D_6 demonstrating the presence of aniline.

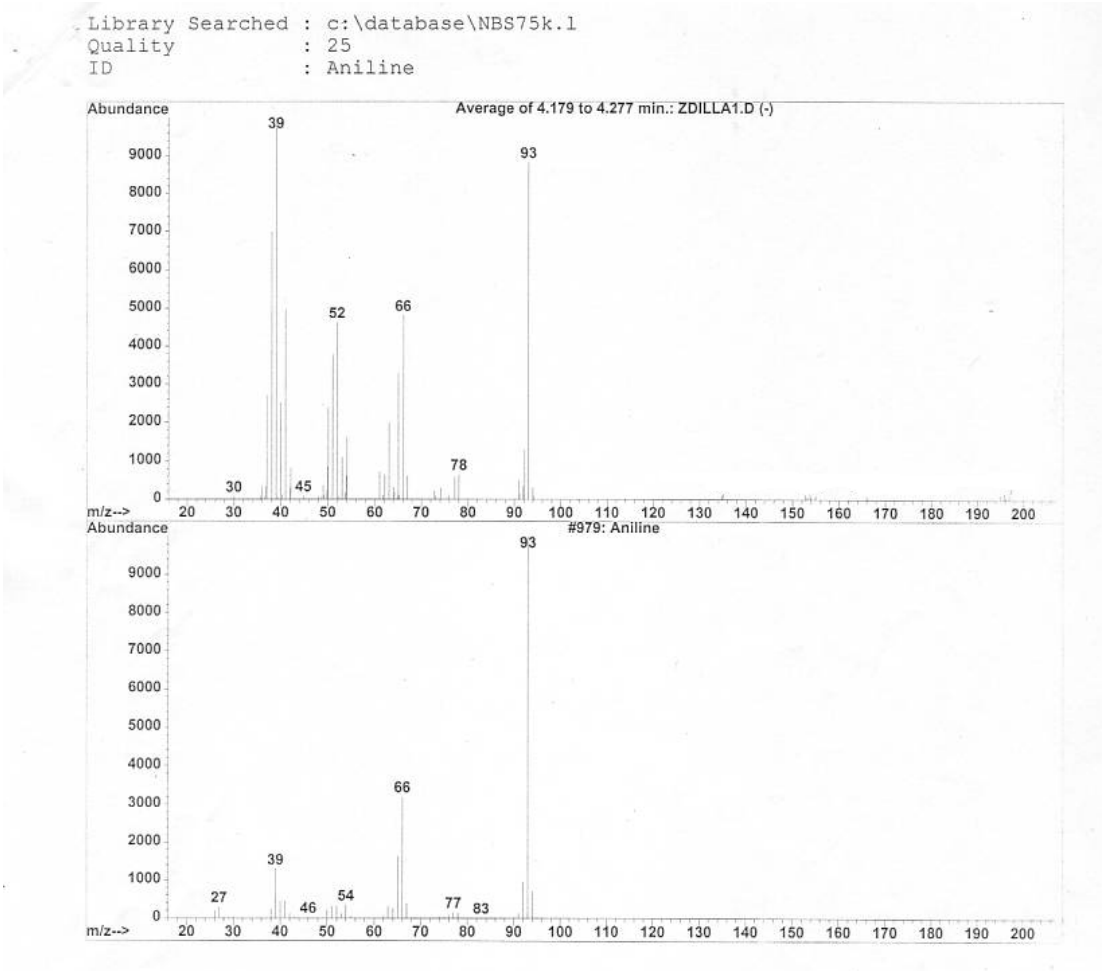

Figure S5. Top: MS of aniline GC-MS peak for pentane wash of filtrate after isolation of **1**. Bottom: Aniline reference spectrum.

FTIR Spectroscopy. The FTIR spectrum of the intermediate from addition of LiNH^{t}Bu to Mn[N(SiMe$_3$)$_2$]$_2$ was recorded in the range of 400-4000 cm1-on a Nicolet Varian Cary 380 FT-IR under nitrogen atmosphere using a KBr pellet press.

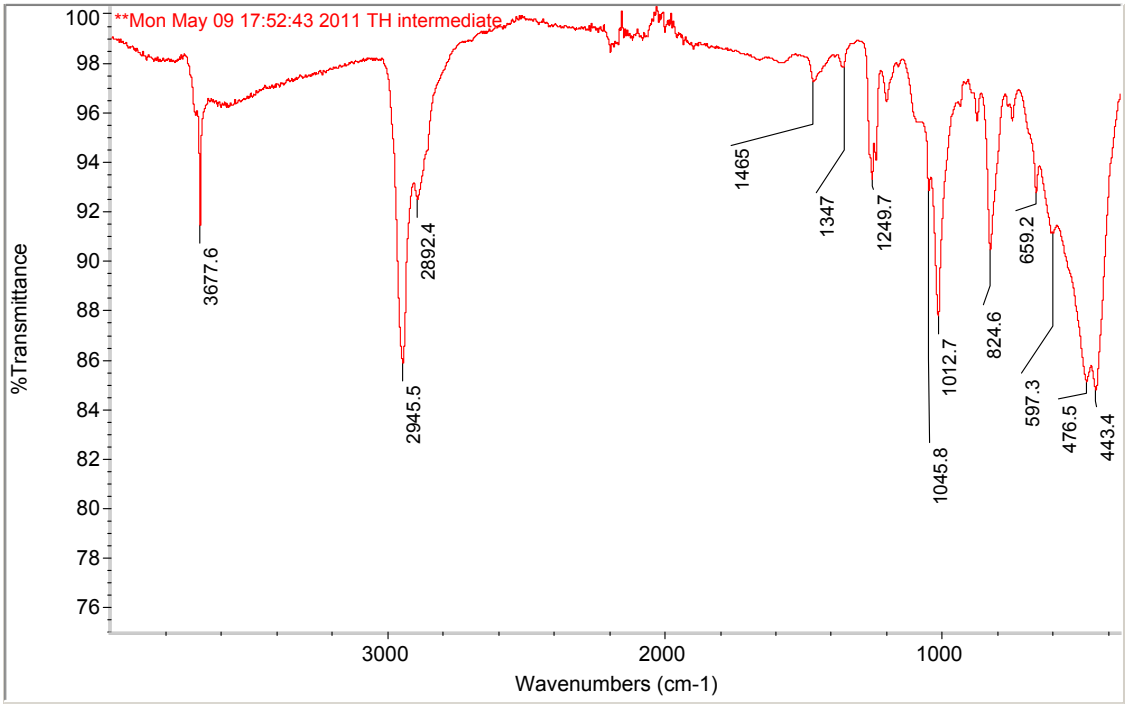

Figure S6. Infrared spectrum of the intermediate addition of LiNH^{t}Bu to Mn[N(SiMe$_3$)$_2$]$_2$. N-H stretch of intermediate amides is seen at 3678 cm^{-1}, and the M=NR stretch of equilibrium terminal imido species is seen at 1250 cm^{-1}.

EPR Spectroscopy EPR Spectra were acquired on a Bruker EMX EPR spectrometer equipped with a liquid He cryostat. Spectra were recorded at 13K. MW power = 20.12 mW. Mod Amplitude = 10.0 dB for Mn[N(SiMe$_3$)$_2$]$_2$ and **1**, Mod. Amplitude = 6 dB for Mn[N(SiMe$_3$)$_2$]$_2$ + LiNH^{t}Bu.

X-Ray Structural Data

Table 1 Selected bond distances (Å) and angles (°)[a] for $Li_2Mn(N_2Ph_2)_3(L)_2$ (L = Et_2O: **1a**, L = THF: **1b**)

	1a	**1b**
Mn(1)-N(1/2/3)	2.0235(18)/1.9656(18)/2.0231(18)	2.0274(11)/1.9685(11)/2.0279(11)
N(1/3)-N(2/3A)	1.413(2)/1.446(3)	1.4173(16)/1.449(2)
N(1/2)…N(3/2A)	2.9266(27)/3.1420(35)	3.1570(24)
Li(1)-N(1/3)	2.037(4)/2.046(5)	2.025(3)2.040(3)
Mn(1)...Li(1)	2.821(4)	2.828(3)
Li(1)-O(1)	1.916(4)	1.902(3)
Li(1)-C(8/14A)	2.771(5)/2.741(5)	2.713(3)/2.749(3)
N(1/3)-Mn(1)-N(2/3A)	41.44(7)/41.88(9)	41.52(5)/41.86(6)
N(1/2)-Mn(1)-N(3/2A)	92.64(8)/106.12(11)	91.83(5)/106.62(7)
N(1/2/2)-Mn(1)-N(3A/3/1A)	106.88(8)/108.99(7)/122.21(8)	106.09(5)/108.85(5)/123.44(5)
N(1/2)-Mn(1)-N(1A/3A)	159.24(11)/142.86(8)	160.96(7)/142.46(5)
N(1)-Li(1)-N(3)	91.56(18)	91.54(12)
N(1/3)-Li(1)-O(1)	135.8(2)/132.4(2)	138.92(16)/129.36(15)
Dihedral Propellar Angles[b]		
Mn(1), N(1,2)	49.1	48.1
Mn(1), N(3,3A)	54.0	54.2

[a] Divided entries refer to separate, related atoms and their associated metrics in the order given, e.g., N(1/2/2)-Mn(1)-N(3A/3/1A) denotes 3 angles, N(1)-Mn(1)-N(3A), N(2)-Mn(1)-N(3), and N(2)-Mn(1)-N(1A). [b] The tilt angle of the "propeller blade" is calculated, for example, as the angle between the N(1)-Mn(1)-N(2) plane and the equatorial molecular plane, the latter fitted (least squares) through all the Mn and N atoms of the complex.

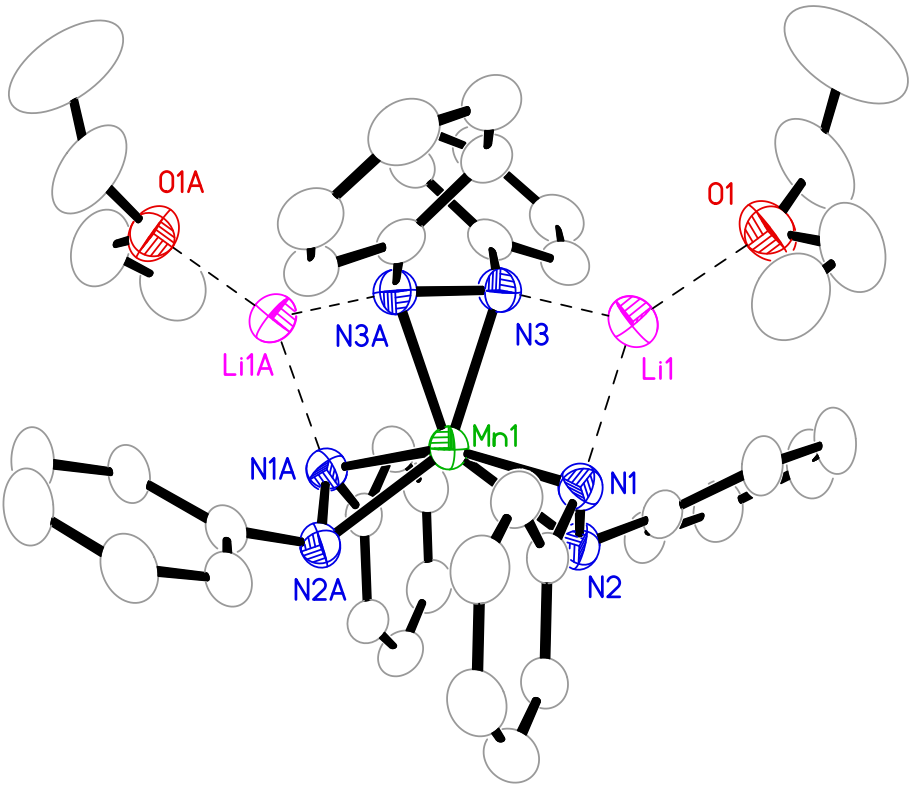

Figure X1. Structure of of $Li_2Mn(N_2Ph_2)_3(Et_2O)_2$ (**1a**) with thermal ellipsoids at 50% probability level. Hydrogen atoms are omitted for clarity.

Table X1.1. Sample and crystal data for 1a.		
Chemical formula	$C_{44}H_{50}Li_2MnN_6O_2$	
Formula weight	763.72	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal size	0.050 x 0.100 x 0.200 mm	
Crystal system	monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 11.9361(15) Å	α = 90°
	b = 18.107(2) Å	β = 96.050(2)°
	c = 19.001(2) Å	γ = 90°
Volume	4083.8(9) $Å^3$	
Z	4	
Density (calculated)	1.242 Mg/cm^3	
Absorption coefficient	0.367 mm^{-1}	
F(000)	1612	

Table X1.2. Data collection and structure refinement for 1a.	
Theta range for data collection	2.16 to 27.48°
Index ranges	-15<=h<=15, -23<=k<=23, -24<=l<=23
Reflections collected	17501
Independent reflections	4676 [R(int) = 0.0184]
Max. and min. transmission	0.9819 and 0.9303
Structure solution technique	direct methods
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-97 (Sheldrick, 2008)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	4676 / 0 / 251
Goodness-of-fit on F^2	1.048
Final R indices	3944 data; $I>2\sigma(I)$ R1 = 0.0544, wR2 = 0.1532
	all data R1 = 0.0647, wR2 = 0.1641
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0859P)^2+7.2898P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.688 and -0.586 eÅ^{-3}
R.M.S. deviation from mean	0.067 eÅ^{-3}

Table X1.3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 1a.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Mn1	0.0	0.04180(2)	0.75	0.02942(16)
N1	0.05792(16)	0.02167(10)	0.65553(10)	0.0317(4)
N2	0.96546(16)	0.97656(10)	0.66790(9)	0.0318(4)
N3	0.95370(14)	0.14615(10)	0.72220(9)	0.0315(4)
Li1	0.0139(4)	0.1270(2)	0.6269(2)	0.0430(9)
O1	0.01188(17)	0.18499(11)	0.54243(10)	0.0516(5)
C1	0.16189(19)	0.98353(12)	0.66302(10)	0.0308(4)
C2	0.2601(2)	0.02580(14)	0.66829(12)	0.0373(5)
C3	0.3647(2)	0.99181(16)	0.67502(13)	0.0436(6)
C4	0.3732(2)	0.91550(16)	0.67596(13)	0.0451(6)
C5	0.2756(2)	0.87348(14)	0.66990(12)	0.0413(5)
C6	0.1707(2)	0.90643(12)	0.66398(11)	0.0347(5)
C7	0.86640(19)	0.99259(13)	0.62390(11)	0.0336(5)
C8	0.8646(2)	0.02716(15)	0.55776(12)	0.0401(5)
C9	0.7625(2)	0.03988(17)	0.51715(14)	0.0510(7)
C10	0.6622(2)	0.0178(2)	0.54065(16)	0.0575(8)
C11	0.6638(2)	0.98216(17)	0.60532(15)	0.0499(7)
C12	0.7641(2)	0.96906(14)	0.64668(12)	0.0390(5)
C13	0.85625(18)	0.17956(12)	0.74247(12)	0.0328(5)
C14	0.8577(2)	0.23110(12)	0.79721(12)	0.0362(5)
C15	0.7582(2)	0.26262(14)	0.81491(14)	0.0435(6)
C16	0.6563(2)	0.24380(16)	0.77851(16)	0.0493(6)
C17	0.6540(2)	0.19387(15)	0.72272(15)	0.0459(6)
C18	0.75160(19)	0.16252(13)	0.70428(14)	0.0390(5)
C19	0.0811(3)	0.1748(3)	0.4866(2)	0.0806(11)
C20	0.1952(4)	0.1464(3)	0.5143(2)	0.0909(13)
C21	0.9127(4)	0.2283(3)	0.5207(3)	0.0986(15)
C22	0.9332(6)	0.2979(4)	0.4998(5)	0.171(3)

Table X1.4. Bond lengths (Å) for 1a.

Mn1-N2#1	1.9656(18)	Mn1-N2	1.9656(18)
Mn1-N3	2.0231(18)	Mn1-N3#1	2.0231(18)
Mn1-N1#1	2.0234(18)	Mn1-N1	2.0235(18)
Mn1-Li1#1	2.821(4)	Mn1-Li1	2.821(4)
N1-N2	1.413(2)	N1-C1	1.414(3)
N1-Li1	2.037(5)	N2-C7	1.405(3)
N3-C13	1.400(3)	N3-N3#1	1.446(3)
N3-Li1	2.046(5)	Li1-O1	1.916(4)
Li1-C14#1	2.741(5)	O1-C19	1.423(4)
O1-C21	1.444(4)	C1-C2	1.395(3)
C1-C6	1.400(3)	C2-C3	1.386(4)
C3-C4	1.385(4)	C4-C5	1.385(4)
C5-C6	1.381(3)	C7-C8	1.402(3)
C7-C12	1.404(3)	C8-C9	1.391(4)
C9-C10	1.380(4)	C10-C11	1.387(4)
C11-C12	1.382(4)	C13-C14	1.396(3)
C13-C18	1.411(3)	C14-C15	1.390(3)
C14-Li1#1	2.741(5)	C15-C16	1.377(4)
C16-C17	1.391(4)	C17-C18	1.374(4)
C19-C20	1.499(6)	C21-C22	1.351(7)

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

Table X1.5. Bond angles (°) for 1a.

N2#1-Mn1-N2	106.12(11)	N2#1-Mn1-N3	142.86(7)
N2-Mn1-N3	108.99(7)	N2#1-Mn1-N3#1	108.99(7)
N2-Mn1-N3#1	142.86(8)	N3-Mn1-N3#1	41.88(9)
N2#1-Mn1-N1#1	41.45(7)	N2-Mn1-N1#1	122.21(8)
N3-Mn1-N1#1	106.88(7)	N3#1-Mn1-N1#1	92.65(8)
N2#1-Mn1-N1	122.21(8)	N2-Mn1-N1	41.45(7)
N3-Mn1-N1	92.64(8)	N3#1-Mn1-N1	106.88(8)
N1#1-Mn1-N1	159.25(11)	N2#1-Mn1-Li1#1	72.34(10)
N2-Mn1-Li1#1	163.92(11)	N3-Mn1-Li1#1	70.56(10)
N3#1-Mn1-Li1#1	46.45(10)	N1#1-Mn1-Li1#1	46.20(10)

Table X1.5. (cont)

N1-Mn1-Li1#1	152.78(11)	N2#1-Mn1-Li1	163.92(11)
N2-Mn1-Li1	72.34(10)	N3-Mn1-Li1	46.45(10)
N3#1-Mn1-Li1	70.56(10)	N1#1-Mn1-Li1	152.78(11)
N1-Mn1-Li1	46.19(10)	Li1#1-Mn1-Li1	113.68(18)
N2-N1-C1	113.17(17)	N2-N1-Mn1	67.08(10)
C1-N1-Mn1	112.15(13)	N2-N1-Li1	113.69(18)
C1-N1-Li1	133.09(19)	Mn1-N1-Li1	88.01(14)
C7-N2-N1	113.89(17)	C7-N2-Mn1	116.18(15)
N1-N2-Mn1	71.47(11)	C13-N3-N3#1	113.1(2)
C13-N3-Mn1	122.92(14)	N3#1-N3-Mn1	69.06(5)
C13-N3-Li1	134.07(18)	N3#1-N3-Li1	109.5(2)
Mn1-N3-Li1	87.77(14)	O1-Li1-N1	135.8(2)
O1-Li1-N3	132.4(2)	N1-Li1-N3	91.56(18)
O1-Li1-C14#1	91.21(18)	N1-Li1-C14#1	112.91(19)
N3-Li1-C14#1	69.36(14)	O1-Li1-Mn1	175.9(2)
N1-Li1-Mn1	45.79(10)	N3-Li1-Mn1	45.77(9)
C14#1-Li1-Mn1	91.07(13)	C19-O1-C21	112.3(3)
C19-O1-Li1	126.6(3)	C21-O1-Li1	118.3(3)
C2-C1-C6	119.0(2)	C2-C1-N1	117.5(2)
C6-C1-N1	123.5(2)	C3-C2-C1	120.3(2)
C4-C3-C2	120.5(2)	C3-C4-C5	119.2(2)
C6-C5-C4	121.1(2)	C5-C6-C1	119.9(2)
C8-C7-C12	118.7(2)	C8-C7-N2	123.9(2)
C12-C7-N2	117.3(2)	C9-C8-C7	120.1(2)
C10-C9-C8	120.8(3)	C9-C10-C11	119.4(3)
C12-C11-C10	120.9(2)	C11-C12-C7	120.2(2)
C14-C13-N3	123.25(19)	C14-C13-C18	118.0(2)
N3-C13-C18	118.7(2)	C15-C14-C13	120.7(2)
C15-C14-Li1#1	126.84(19)	C13-C14-Li1#1	83.94(15)
C16-C15-C14	120.6(2)	C15-C16-C17	119.3(2)
C18-C17-C16	120.9(2)	C17-C18-C13	120.5(2)
O1-C19-C20	111.1(3)	C22-C21-O1	115.0(5)

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

Table X1.6. Torsion angles (°) for 1a.

N2#1-Mn1-N1-N2	77.42(17)	N3-Mn1-N1-N2	-116.10(11)
N3#1-Mn1-N1-N2	-156.20(11)	N1#1-Mn1-N1-N2	44.30(10)
Li1#1-Mn1-N1-N2	-166.4(2)	Li1-Mn1-N1-N2	-116.82(18)
N2#1-Mn1-N1-C1	-29.39(17)	N2-Mn1-N1-C1	-106.81(18)
N3-Mn1-N1-C1	137.09(14)	N3#1-Mn1-N1-C1	96.98(15)
N1#1-Mn1-N1-C1	-62.51(14)	Li1#1-Mn1-N1-C1	86.8(3)
Li1-Mn1-N1-C1	136.4(2)	N2#1-Mn1-N1-Li1	-165.77(15)
N2-Mn1-N1-Li1	116.82(18)	N3-Mn1-N1-Li1	0.72(14)
N3#1-Mn1-N1-Li1	-39.39(15)	N1#1-Mn1-N1-Li1	161.12(14)
Li1#1-Mn1-N1-Li1	-49.6(4)	C1-N1-N2-C7	-143.55(18)
Mn1-N1-N2-C7	111.13(17)	Li1-N1-N2-C7	34.2(2)
C1-N1-N2-Mn1	105.32(15)	Li1-N1-N2-Mn1	-76.90(16)
N2#1-Mn1-N2-C7	131.13(17)	N3-Mn1-N2-C7	-36.56(17)
N3#1-Mn1-N2-C7	-68.4(2)	N1#1-Mn1-N2-C7	88.88(16)
N1-Mn1-N2-C7	-108.13(19)	Li1#1-Mn1-N2-C7	49.0(4)
Li1-Mn1-N2-C7	-65.60(17)	N2#1-Mn1-N2-N1	-120.74(12)
N3-Mn1-N2-N1	71.57(12)	N3#1-Mn1-N2-N1	39.75(17)
N1#1-Mn1-N2-N1	-162.99(9)	Li1#1-Mn1-N2-N1	157.2(4)
Li1-Mn1-N2-N1	42.53(13)	N2#1-Mn1-N3-C13	-56.3(2)
N2-Mn1-N3-C13	103.85(17)	N3#1-Mn1-N3-C13	-104.6(2)
N1#1-Mn1-N3-C13	-30.06(17)	N1-Mn1-N3-C13	142.80(16)
Li1#1-Mn1-N3-C13	-59.11(18)	Li1-Mn1-N3-C13	143.5(2)
N2#1-Mn1-N3-N3#1	48.3(2)	N2-Mn1-N3-N3#1	-151.52(14)
N1#1-Mn1-N3-N3#1	74.57(16)	N1-Mn1-N3-N3#1	-112.57(15)
Li1#1-Mn1-N3-N3#1	45.51(16)	Li1-Mn1-N3-N3#1	-111.9(2)
N2#1-Mn1-N3-Li1	160.17(16)	N2-Mn1-N3-Li1	-39.66(15)
N3#1-Mn1-N3-Li1	111.9(2)	N1#1-Mn1-N3-Li1	-173.58(14)
N1-Mn1-N3-Li1	-0.71(14)	Li1#1-Mn1-N3-Li1	157.37(10)
N2-N1-Li1-O1	-110.8(3)	C1-N1-Li1-O1	66.4(4)
Mn1-N1-Li1-O1	-174.7(3)	N2-N1-Li1-N3	63.1(2)
C1-N1-Li1-N3	-119.7(2)	Mn1-N1-Li1-N3	-0.71(14)
N2-N1-Li1-C14#1	131.34(18)	C1-N1-Li1-C14#1	-51.5(3)
Mn1-N1-Li1-C14#1	67.49(17)	N2-N1-Li1-Mn1	63.85(13)
C1-N1-Li1-Mn1	-119.0(2)	C13-N3-Li1-O1	39.0(5)
N3#1-N3-Li1-O1	-118.1(3)	Mn1-N3-Li1-O1	175.0(3)
C13-N3-Li1-N1	-135.3(2)	N3#1-N3-Li1-N1	67.56(16)

Table X1.6 (cont)

Mn1-N3-Li1-N1	0.71(14)	C13-N3-Li1-C14#1	110.8(2)
N3#1-N3-Li1-C14#1	-46.38(10)	Mn1-N3-Li1-C14#1	-113.23(9)
C13-N3-Li1-Mn1	-136.0(2)	N3#1-N3-Li1-Mn1	66.85(6)
N2#1-Mn1-Li1-O1	163.(3)	N2-Mn1-Li1-O1	76.(3)
N3-Mn1-Li1-O1	-65.(3)	N3#1-Mn1-Li1-O1	-106.(3)
N1#1-Mn1-Li1-O1	-51.(3)	N1-Mn1-Li1-O1	114.(3)
Li1#1-Mn1-Li1-O1	-88.(3)	N2#1-Mn1-Li1-N1	48.7(4)
N2-Mn1-Li1-N1	-38.31(11)	N3-Mn1-Li1-N1	-179.0(2)
N3#1-Mn1-Li1-N1	139.91(15)	N1#1-Mn1-Li1-N1	-165.48(13)
Li1#1-Mn1-Li1-N1	157.65(16)	N2#1-Mn1-Li1-N3	-132.3(3)
N2-Mn1-Li1-N3	140.70(14)	N3#1-Mn1-Li1-N3	-41.08(13)
N1#1-Mn1-Li1-N3	13.5(3)	N1-Mn1-Li1-N3	179.0(2)
Li1#1-Mn1-Li1-N3	-23.34(8)	N2#1-Mn1-Li1-C14#1	-73.0(4)
N2-Mn1-Li1-C14#1	-159.98(15)	N3-Mn1-Li1-C14#1	59.32(12)
N3#1-Mn1-Li1-C14#1	18.25(10)	N1#1-Mn1-Li1-C14#1	72.9(3)
N1-Mn1-Li1-C14#1	-121.67(18)	Li1#1-Mn1-Li1-C14#1	35.98(8)
N1-Li1-O1-C19	-26.0(5)	N3-Li1-O1-C19	162.2(3)
C14#1-Li1-O1-C19	99.5(3)	Mn1-Li1-O1-C19	-137.(3)
N1-Li1-O1-C21	133.9(4)	N3-Li1-O1-C21	-37.9(5)
C14#1-Li1-O1-C21	-100.7(3)	Mn1-Li1-O1-C21	23.(3)
N2-N1-C1-C2	-165.42(18)	Mn1-N1-C1-C2	-91.9(2)
Li1-N1-C1-C2	17.4(3)	N2-N1-C1-C6	15.9(3)
Mn1-N1-C1-C6	89.4(2)	Li1-N1-C1-C6	-161.4(2)
C6-C1-C2-C3	-0.6(3)	N1-C1-C2-C3	-179.4(2)
C1-C2-C3-C4	0.6(4)	C2-C3-C4-C5	0.2(4)
C3-C4-C5-C6	-0.9(4)	C4-C5-C6-C1	0.9(3)
C2-C1-C6-C5	-0.2(3)	N1-C1-C6-C5	178.5(2)
N1-N2-C7-C8	23.7(3)	Mn1-N2-C7-C8	103.9(2)
N1-N2-C7-C12	-159.53(19)	Mn1-N2-C7-C12	-79.3(2)
C12-C7-C8-C9	2.2(4)	N2-C7-C8-C9	179.0(2)
C7-C8-C9-C10	-1.0(4)	C8-C9-C10-C11	-0.4(5)
C9-C10-C11-C12	0.6(5)	C10-C11-C12-C7	0.7(4)
C8-C7-C12-C11	-2.1(4)	N2-C7-C12-C11	-179.1(2)
N3#1-N3-C13-C14	23.1(3)	Mn1-N3-C13-C14	102.4(2)
Li1-N3-C13-C14	-133.4(3)	N3#1-N3-C13-C18	-159.21(17)
Mn1-N3-C13-C18	-80.0(2)	Li1-N3-C13-C18	44.3(3)
N3-C13-C14-C15	179.8(2)	C18-C13-C14-C15	2.2(3)

Table X1.6 (cont)

N3-C13-C14-Li1#1	-50.5(2)	C18-C13-C14-Li1#1	131.8(2)
C13-C14-C15-C16	-0.3(4)	Li1#1-C14-C15-C16	-107.3(3)
C14-C15-C16-C17	-1.3(4)	C15-C16-C17-C18	0.9(4)
C16-C17-C18-C13	1.0(4)	C14-C13-C18-C17	-2.5(3)
N3-C13-C18-C17	179.7(2)	C21-O1-C19-C20	166.1(4)
Li1-O1-C19-C20	-33.0(5)	C19-O1-C21-C22	-61.8(7)
Li1-O1-C21-C22	135.6(6)		

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

Table X1.7. Anisotropic atomic displacement parameters (Å^2) for 1a.

The anisotropic atomic displacement factor exponent takes the form:
$-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mn1	0.0324(3)	0.0286(2)	0.0260(2)	0	-0.00264(17)	0
N1	0.0338(9)	0.0311(9)	0.0293(9)	0.0009(7)	-0.0003(7)	-0.0042(7)
N2	0.0356(10)	0.0332(9)	0.0259(8)	0.0000(7)	0.0003(7)	-0.0064(7)
N3	0.0279(9)	0.0301(9)	0.0344(9)	0.0010(7)	-0.0072(7)	-0.0007(7)
Li1	0.055(2)	0.038(2)	0.036(2)	0.0053(16)	0.0012(17)	-0.0005(18)
O1	0.0563(11)	0.0503(11)	0.0465(10)	0.0117(8)	-0.0027(8)	-0.0007(9)
C1	0.0366(11)	0.0339(10)	0.0218(9)	0.0004(8)	0.0029(8)	-0.0013(9)
C2	0.0407(12)	0.0391(12)	0.0323(11)	-0.0026(9)	0.0044(9)	-0.0030(9)
C3	0.0367(12)	0.0531(15)	0.0409(13)	-0.0027(11)	0.0041(10)	-0.0036(11)
C4	0.0420(13)	0.0549(15)	0.0391(13)	0.0039(11)	0.0075(10)	0.0101(11)
C5	0.0530(14)	0.0377(12)	0.0343(11)	0.0056(9)	0.0101(10)	0.0077(10)
C6	0.0432(12)	0.0338(11)	0.0276(10)	0.0027(8)	0.0063(9)	-0.0009(9)
C7	0.0377(11)	0.0356(11)	0.0267(10)	-0.0035(8)	-0.0012(8)	-0.0079(9)
C8	0.0392(12)	0.0533(14)	0.0270(11)	-0.0009(9)	-0.0001(9)	-0.0136(10)
C9	0.0491(15)	0.0702(19)	0.0311(12)	0.0056(11)	-0.0080(11)	-0.0145(13)
C10	0.0423(14)	0.082(2)	0.0450(15)	0.0041(14)	-0.0126(11)	-0.0160(14)
C11	0.0378(13)	0.0661(17)	0.0454(14)	-0.0036(13)	0.0024(11)	-0.0196(12)
C12	0.0436(13)	0.0444(13)	0.0289(11)	-0.0024(9)	0.0030(9)	-0.0140(10)
C13	0.0310(10)	0.0280(10)	0.0377(11)	0.0087(8)	-0.0044(8)	-0.0016(8)
C14	0.0359(11)	0.0320(11)	0.0390(12)	0.0048(9)	-0.0044(9)	0.0018(9)
C15	0.0473(14)	0.0387(12)	0.0442(13)	0.0045(10)	0.0041(10)	0.0070(10)
C16	0.0350(12)	0.0521(15)	0.0613(16)	0.0109(13)	0.0077(11)	0.0072(11)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C17	0.0310(11)	0.0449(14)	0.0600(16)	0.0101(12)	-0.0045(10)	-0.0029(10)
C18	0.0332(11)	0.0347(11)	0.0466(13)	0.0066(10)	-0.0076(9)	-0.0031(9)
C19	0.082(3)	0.104(3)	0.056(2)	0.018(2)	0.0121(18)	0.005(2)
C20	0.111(3)	0.092(3)	0.071(2)	-0.016(2)	0.017(2)	0.008(3)
C21	0.079(3)	0.120(4)	0.095(3)	0.049(3)	0.002(2)	0.027(3)
C22	0.157(6)	0.134(6)	0.223(9)	0.091(6)	0.018(6)	0.042(5)

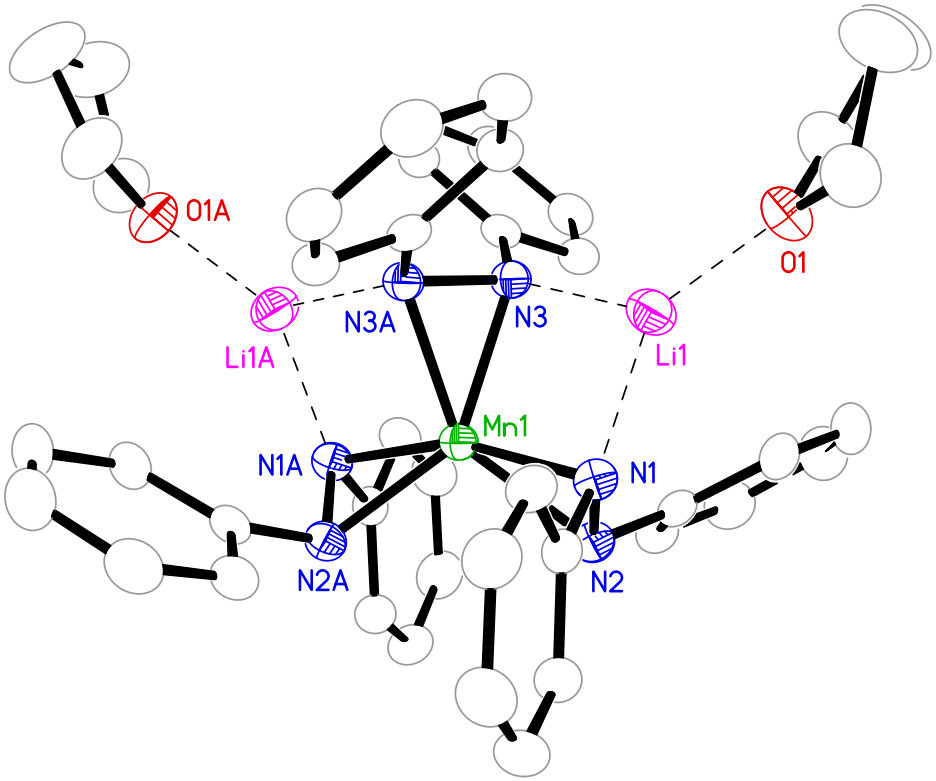

Figure X2. Structure of of $Li_2Mn(N_2Ph_2)_3(Et_2O)_2$ (**1a**) with thermal ellipsoids at 50% probability level. Hydrogen atoms are omitted for clarity.

Table X2.1. Sample and crystal data for 1b.	
Chemical formula	$C_{44}H_{46}Li_2MnN_6O_2$
Formula weight	759.69
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal size	0.080 x 0.150 x 0.200 mm
Crystal system	monoclinic
Space group	C 1 2/c 1
Unit cell dimensions	a = 12.0250(7) Å α = 90°
	b = 17.5310(10) Å β = 95.1030(10)°
	c = 18.7595(11) Å γ = 90°
Volume	3939.0(4) $Å^3$
Z	4
Density (calculated)	1.281 Mg/cm^3
Absorption coefficient	0.380 mm^{-1}
F(000)	1596

Table X2.2. Data collection and structure refinement for 1b.	
Theta range for data collection	2.06 to 27.88°
Index ranges	-15<=h<=15, -22<=k<=23, -24<=l<=24
Reflections collected	18662
Independent reflections	4676 [R(int) = 0.0253]
Max. and min. transmission	0.9702 and 0.9279
Structure solution technique	direct methods
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-97 (Sheldrick, 2008)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	4676 / 0 / 249
Goodness-of-fit on F^2	1.025
Δ/σ_{max}	0.001
Final R indices	3858 data; I>2σ(I) R1 = 0.0341, wR2 = 0.0835
	all data R1 = 0.0468, wR2 = 0.0897
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0394P)^2+3.4189P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.375 and -0.259 $eÅ^{-3}$
R.M.S. deviation from mean	0.044 $eÅ^{-3}$

Table X2.3. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 1b.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
Mn1	0.0	0.023238(16)	0.75	0.02051(9)
Li1	0.0089(2)	0.11120(15)	0.62425(15)	0.0336(6)
N3	0.95397(9)	0.13128(6)	0.72233(6)	0.0219(2)
N2	0.96663(10)	0.95615(7)	0.66670(6)	0.0232(2)
N1	0.05727(10)	0.00411(7)	0.65315(6)	0.0229(2)
O1	0.99919(10)	0.17440(7)	0.54152(6)	0.0366(3)
C21	0.0625(2)	0.28022(13)	0.48265(14)	0.0693(7)
C7	0.86725(11)	0.97313(8)	0.62435(7)	0.0227(3)
C1	0.16131(11)	0.96589(8)	0.65943(7)	0.0224(3)
C8	0.86257(13)	0.01041(9)	0.55821(8)	0.0272(3)
C3	0.36225(13)	0.97722(10)	0.66988(9)	0.0333(3)
C2	0.25780(12)	0.01095(9)	0.66332(8)	0.0271(3)
C12	0.76707(13)	0.94785(9)	0.64966(8)	0.0281(3)
C13	0.85593(11)	0.16352(8)	0.74408(8)	0.0220(3)
C9	0.76032(14)	0.02484(10)	0.52011(9)	0.0354(4)
C15	0.75401(13)	0.24472(9)	0.82015(9)	0.0313(3)
C6	0.17220(13)	0.88662(8)	0.66048(8)	0.0268(3)
C14	0.85443(12)	0.21507(8)	0.80132(8)	0.0259(3)
C17	0.65487(12)	0.17511(9)	0.72522(9)	0.0306(3)
C18	0.75386(12)	0.14504(8)	0.70559(8)	0.0255(3)
C5	0.27751(13)	0.85381(9)	0.66646(8)	0.0319(3)
C11	0.66641(13)	0.96200(10)	0.61045(10)	0.0362(4)
C16	0.65396(13)	0.22490(10)	0.78294(9)	0.0340(4)
C10	0.66242(14)	0.00133(11)	0.54615(10)	0.0415(4)
C4	0.37273(13)	0.89836(10)	0.67171(9)	0.0358(4)
C22	0.08426(17)	0.19763(11)	0.49683(11)	0.0466(5)
C19	0.90241(17)	0.22097(12)	0.52391(12)	0.0511(5)
C20	0.9386(2)	0.28762(14)	0.48342(15)	0.0749(8)

Table X2.4. Bond lengths (Å) for 1b.

Mn1-N2	1.9685(12)	Mn1-N2#1	1.9685(12)
Mn1-N1#1	2.0273(12)	Mn1-N1	2.0274(12)
Mn1-N3	2.0279(12)	Mn1-N3#1	2.0280(12)
Mn1-Li1#1	2.828(3)	Li1-O1	1.902(3)
Li1-N1	2.025(3)	Li1-N3	2.040(3)
Li1-C14#1	2.749(3)	N3-C13	1.4004(17)
N3-N3#1	1.449(2)	N2-C7	1.4067(18)
N2-N1	1.4173(16)	N1-C1	1.4149(18)
O1-C19	1.436(2)	O1-C22	1.438(2)
C21-C22	1.491(3)	C21-C20	1.498(4)
C7-C8	1.399(2)	C7-C12	1.405(2)
C1-C6	1.396(2)	C1-C2	1.400(2)
C8-C9	1.389(2)	C3-C2	1.384(2)
C3-C4	1.388(2)	C12-C11	1.382(2)
C13-C14	1.405(2)	C13-C18	1.4054(19)
C9-C10	1.377(2)	C15-C16	1.381(2)
C15-C14	1.389(2)	C6-C5	1.386(2)
C14-Li1#1	2.749(3)	C17-C18	1.381(2)
C17-C16	1.392(2)	C5-C4	1.382(2)
C11-C10	1.386(3)	C19-C20	1.480(3)

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

Table X2.5. Bond angles (°) for 1b.

N2-Mn1-N2#1	106.62(7)	N2-Mn1-N1#1	123.44(5)
N2#1-Mn1-N1#1	41.52(5)	N2-Mn1-N1	41.52(5)
N2#1-Mn1-N1	123.44(5)	N1#1-Mn1-N1	160.96(7)
N2-Mn1-N3	108.85(5)	N2#1-Mn1-N3	142.47(5)
N1#1-Mn1-N3	106.09(5)	N1-Mn1-N3	91.83(5)
N2-Mn1-N3#1	142.46(5)	N2#1-Mn1-N3#1	108.86(5)
N1#1-Mn1-N3#1	91.83(5)	N1-Mn1-N3#1	106.09(5)
N3-Mn1-N3#1	41.86(6)	N2-Mn1-Li1#1	165.42(7)
N2#1-Mn1-Li1#1	71.57(7)	N1#1-Mn1-Li1#1	45.71(6)
N1-Mn1-Li1#1	151.48(7)	N3-Mn1-Li1#1	71.00(7)

Table X2.5 (cont)

N3#1-Mn1-Li1#1	46.13(6)	O1-Li1-N1	138.92(16)
O1-Li1-N3	129.36(15)	N1-Li1-N3	91.54(12)
O1-Li1-C14#1	91.09(11)	N1-Li1-C14#1	109.48(12)
N3-Li1-C14#1	69.79(9)	C13-N3-N3#1	113.62(13)
C13-N3-Mn1	121.33(9)	N3#1-N3-Mn1	69.07(3)
C13-N3-Li1	132.91(12)	N3#1-N3-Li1	110.99(13)
Mn1-N3-Li1	88.10(9)	C7-N2-N1	113.67(11)
C7-N2-Mn1	115.14(9)	N1-N2-Mn1	71.47(7)
C1-N1-N2	113.11(11)	C1-N1-Li1	133.80(12)
N2-N1-Li1	113.00(12)	C1-N1-Mn1	111.84(9)
N2-N1-Mn1	67.02(7)	Li1-N1-Mn1	88.52(9)
C19-O1-C22	107.99(14)	C19-O1-Li1	120.56(14)
C22-O1-Li1	130.21(14)	C22-C21-C20	103.96(19)
C8-C7-C12	118.61(13)	C8-C7-N2	124.39(13)
C12-C7-N2	116.95(13)	C6-C1-C2	119.00(13)
C6-C1-N1	123.62(13)	C2-C1-N1	117.37(13)
C9-C8-C7	120.35(14)	C2-C3-C4	120.49(15)
C3-C2-C1	120.33(14)	C11-C12-C7	120.02(15)
N3-C13-C14	123.41(12)	N3-C13-C18	118.46(13)
C14-C13-C18	118.11(13)	C10-C9-C8	120.55(16)
C16-C15-C14	121.03(15)	C5-C6-C1	119.88(14)
C15-C14-C13	120.38(14)	C15-C14-Li1#1	127.78(12)
C13-C14-Li1#1	85.09(10)	C18-C17-C16	120.89(14)
C17-C18-C13	120.59(14)	C4-C5-C6	121.08(15)
C12-C11-C10	120.88(15)	C15-C16-C17	118.98(14)
C9-C10-C11	119.53(15)	C5-C4-C3	119.22(14)
O1-C22-C21	104.86(16)	O1-C19-C20	107.33(17)
C19-C20-C21	105.94(18)		

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

Table X2.6. Torsion angles (°) for 1b.

N2-Mn1-N3-C13	103.37(11)	N2#1-Mn1-N3-C13	-56.77(13)
N1#1-Mn1-N3-C13	-31.43(11)	N1-Mn1-N3-C13	142.04(10)
N3#1-Mn1-N3-C13	-105.63(15)	Li1#1-Mn1-N3-C13	-61.21(11)
N2-Mn1-N3-N3#1	-151.00(9)	N2#1-Mn1-N3-N3#1	48.86(13)
N1#1-Mn1-N3-N3#1	74.21(10)	N1-Mn1-N3-N3#1	-112.32(9)
Li1#1-Mn1-N3-N3#1	44.42(10)	N2-Mn1-N3-Li1	-37.64(10)
N2#1-Mn1-N3-Li1	162.21(10)	N1#1-Mn1-N3-Li1	-172.44(9)
N1-Mn1-N3-Li1	1.03(9)	N3#1-Mn1-N3-Li1	113.35(13)
Li1#1-Mn1-N3-Li1	157.78(6)	O1-Li1-N3-C13	42.0(3)
N1-Li1-N3-C13	-133.83(13)	C14#1-Li1-N3-C13	115.95(14)
O1-Li1-N3-N3#1	-118.54(18)	N1-Li1-N3-N3#1	65.67(11)
C14#1-Li1-N3-N3#1	-44.55(7)	O1-Li1-N3-Mn1	174.76(19)
N1-Li1-N3-Mn1	-1.03(9)	C14#1-Li1-N3-Mn1	-111.25(6)
N2#1-Mn1-N2-C7	129.88(11)	N1#1-Mn1-N2-C7	87.55(11)
N1-Mn1-N2-C7	-108.08(12)	N3-Mn1-N2-C7	-37.65(11)
N3#1-Mn1-N2-C7	-69.72(12)	Li1#1-Mn1-N2-C7	49.3(3)
N2#1-Mn1-N2-N1	-122.04(8)	N1#1-Mn1-N2-N1	-164.37(6)
N3-Mn1-N2-N1	70.43(8)	N3#1-Mn1-N2-N1	38.36(11)
Li1#1-Mn1-N2-N1	157.4(3)	C7-N2-N1-C1	-145.01(12)
Mn1-N2-N1-C1	104.97(10)	C7-N2-N1-Li1	32.17(16)
Mn1-N2-N1-Li1	-77.85(11)	C7-N2-N1-Mn1	110.02(10)
O1-Li1-N1-C1	66.6(3)	N3-Li1-N1-C1	-118.37(15)
C14#1-Li1-N1-C1	-49.3(2)	O1-Li1-N1-N2	-109.8(2)
N3-Li1-N1-N2	65.23(14)	C14#1-Li1-N1-N2	134.30(11)
O1-Li1-N1-Mn1	-174.0(2)	N3-Li1-N1-Mn1	1.03(9)
C14#1-Li1-N1-Mn1	70.11(10)	N2-Mn1-N1-C1	-106.82(12)
N2#1-Mn1-N1-C1	-30.06(11)	N1#1-Mn1-N1-C1	-63.25(9)
N3-Mn1-N1-C1	136.32(9)	N3#1-Mn1-N1-C1	96.35(9)
Li1#1-Mn1-N1-C1	84.89(17)	N2#1-Mn1-N1-N2	76.76(11)
N1#1-Mn1-N1-N2	43.57(6)	N3-Mn1-N1-N2	-116.86(7)
N3#1-Mn1-N1-N2	-156.83(7)	Li1#1-Mn1-N1-N2	-168.29(14)
N2-Mn1-N1-Li1	115.82(11)	N2#1-Mn1-N1-Li1	-167.42(9)
N1#1-Mn1-N1-Li1	159.39(9)	N3-Mn1-N1-Li1	-1.04(9)
N3#1-Mn1-N1-Li1	-41.01(10)	Li1#1-Mn1-N1-Li1	-52.5(2)
N1-Li1-O1-C19	136.9(2)	N3-Li1-O1-C19	-36.7(3)
C14#1-Li1-O1-C19	-101.13(16)	N1-Li1-O1-C22	-57.4(3)

Table X2.6 (cont)

N3-Li1-O1-C22	129.0(2)	C14#1-Li1-O1-C22	64.56(18)
N1-N2-C7-C8	23.72(19)	Mn1-N2-C7-C8	103.49(14)
N1-N2-C7-C12	-158.91(12)	Mn1-N2-C7-C12	-79.14(14)
N2-N1-C1-C6	15.52(19)	Li1-N1-C1-C6	-160.88(16)
Mn1-N1-C1-C6	88.88(14)	N2-N1-C1-C2	-165.79(12)
Li1-N1-C1-C2	17.8(2)	Mn1-N1-C1-C2	-92.43(13)
C12-C7-C8-C9	2.7(2)	N2-C7-C8-C9	-179.94(14)
C4-C3-C2-C1	0.9(2)	C6-C1-C2-C3	-1.6(2)
N1-C1-C2-C3	179.67(13)	C8-C7-C12-C11	-1.9(2)
N2-C7-C12-C11	-179.46(14)	N3#1-N3-C13-C14	22.34(16)
Mn1-N3-C13-C14	101.38(14)	Li1-N3-C13-C14	-137.76(16)
N3#1-N3-C13-C18	-159.41(10)	Mn1-N3-C13-C18	-80.37(14)
Li1-N3-C13-C18	40.5(2)	C7-C8-C9-C10	-1.3(2)
C2-C1-C6-C5	1.0(2)	N1-C1-C6-C5	179.69(13)
C16-C15-C14-C13	-0.6(2)	C16-C15-C14-Li1#1	-109.77(18)
N3-C13-C14-C15	-179.83(13)	C18-C13-C14-C15	1.9(2)
N3-C13-C14-Li1#1	-48.34(14)	C18-C13-C14-Li1#1	133.41(13)
C16-C17-C18-C13	0.7(2)	N3-C13-C18-C17	179.68(13)
C14-C13-C18-C17	-2.0(2)	C1-C6-C5-C4	0.3(2)
C7-C12-C11-C10	-0.3(2)	C14-C15-C16-C17	-0.8(2)
C18-C17-C16-C15	0.7(2)	C8-C9-C10-C11	-0.9(3)
C12-C11-C10-C9	1.7(3)	C6-C5-C4-C3	-1.0(3)
C2-C3-C4-C5	0.4(3)	C19-O1-C22-C21	29.8(2)
Li1-O1-C22-C21	-137.3(2)	C20-C21-C22-O1	-31.1(2)
C22-O1-C19-C20	-16.3(2)	Li1-O1-C19-C20	152.31(19)
O1-C19-C20-C21	-3.7(3)	C22-C21-C20-C19	21.2(3)

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

Table X2.7. Anisotropic atomic displacement parameters (Å^2) for 1b.

The anisotropic atomic displacement factor exponent takes the form:
$-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mn1	0.01953(15)	0.01932(15)	0.02259(16)	0	0.00131(11)	0
Li1	0.0393(15)	0.0289(13)	0.0329(14)	0.0045(11)	0.0046(12)	0.0050(11)
N3	0.0181(6)	0.0205(6)	0.0263(6)	-0.0005(5)	-0.0019(5)	0.0000(4)
N2	0.0203(6)	0.0235(6)	0.0257(6)	-0.0012(5)	0.0023(5)	-0.0019(4)
N1	0.0203(6)	0.0230(6)	0.0258(6)	-0.0009(5)	0.0031(5)	-0.0010(4)
O1	0.0377(6)	0.0378(6)	0.0344(6)	0.0102(5)	0.0036(5)	0.0031(5)
C21	0.0911(19)	0.0494(13)	0.0710(16)	0.0176(11)	0.0264(14)	-0.0061(12)
C7	0.0234(7)	0.0206(6)	0.0241(7)	-0.0062(5)	0.0017(5)	-0.0007(5)
C1	0.0227(7)	0.0257(7)	0.0193(6)	-0.0016(5)	0.0043(5)	0.0021(5)
C8	0.0264(7)	0.0318(8)	0.0236(7)	-0.0045(6)	0.0039(6)	-0.0030(6)
C3	0.0229(7)	0.0393(9)	0.0384(9)	-0.0034(7)	0.0057(6)	-0.0006(6)
C2	0.0253(7)	0.0261(7)	0.0302(8)	-0.0035(6)	0.0041(6)	0.0001(6)
C12	0.0288(8)	0.0264(7)	0.0293(8)	-0.0026(6)	0.0040(6)	-0.0051(6)
C13	0.0208(6)	0.0180(6)	0.0271(7)	0.0043(5)	0.0011(5)	0.0005(5)
C9	0.0371(9)	0.0412(9)	0.0266(8)	0.0002(7)	-0.0053(7)	-0.0032(7)
C15	0.0347(8)	0.0270(8)	0.0324(8)	-0.0017(6)	0.0040(6)	0.0060(6)
C6	0.0286(7)	0.0255(7)	0.0268(7)	-0.0001(6)	0.0059(6)	0.0005(6)
C14	0.0246(7)	0.0230(7)	0.0294(8)	0.0003(6)	-0.0019(6)	0.0015(5)
C17	0.0211(7)	0.0317(8)	0.0382(9)	0.0052(7)	-0.0013(6)	0.0011(6)
C18	0.0239(7)	0.0222(7)	0.0297(8)	0.0011(6)	-0.0008(6)	0.0004(5)
C5	0.0365(9)	0.0273(8)	0.0332(8)	0.0021(6)	0.0099(7)	0.0081(6)
C11	0.0243(8)	0.0387(9)	0.0457(10)	-0.0031(7)	0.0032(7)	-0.0085(6)
C16	0.0257(8)	0.0361(9)	0.0410(9)	0.0039(7)	0.0077(7)	0.0078(6)
C10	0.0279(8)	0.0487(10)	0.0453(10)	-0.0004(8)	-0.0113(7)	-0.0038(7)
C4	0.0269(8)	0.0418(9)	0.0395(9)	0.0026(7)	0.0073(7)	0.0112(7)
C22	0.0510(11)	0.0491(11)	0.0421(10)	0.0035(8)	0.0175(9)	0.0026(9)
C19	0.0458(11)	0.0547(12)	0.0531(12)	0.0114(9)	0.0057(9)	0.0135(9)
C20	0.0844(18)	0.0552(14)	0.0855(18)	0.0321(13)	0.0096(14)	0.0193(13)