Synthesis and Crystallographic Characterization of New Mn(I) Complexes of Donor-Functionalized Indenes

Judy Cipot,[a] Dominik Wechsler,[a] Robert McDonald,[b] Michael J. Ferguson,[b] and Mark Stradiotto*[a]

[a]Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada B3H 4J3. Fax: 1-902-494-1310; Tel: 1-902-494-7190; E-mail: mark.stradiotto@dal.ca
[b]X-Ray Crystallography Laboratory, Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada T6G 2G2.

SUPPORTING INFORMATION

Contents:

Contents (continued):

Contents (continued):

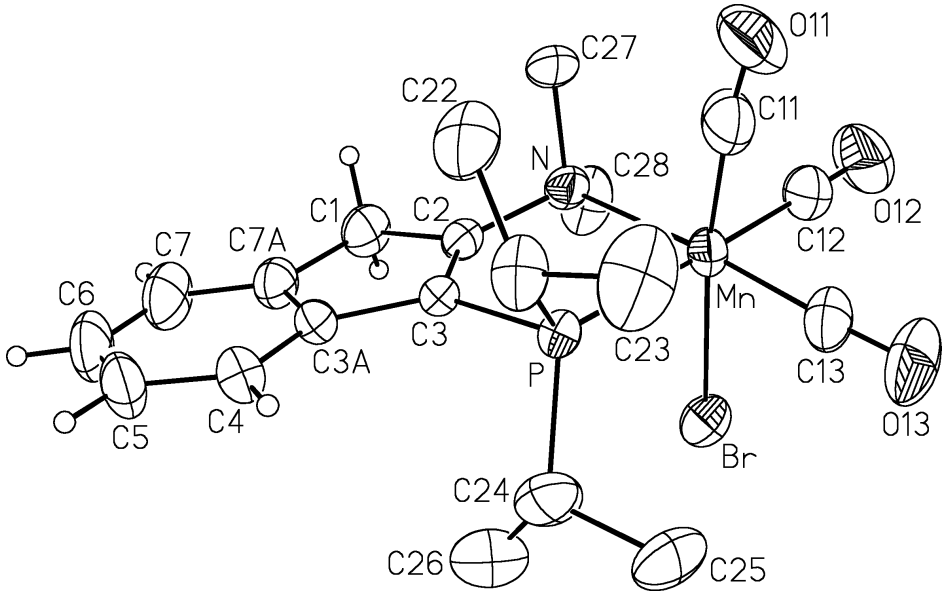

Figure 1a. Perspective view of the [{κ^2–(2-Me$_2$N-1*H*-inden-3-yl)P^{i}Pr$_2$}MnBr(CO)$_3$] molecule showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 50% probability level. Hydrogen atoms are shown with arbitrarily small thermal parameters for the indenyl group; all other hydrogens are not shown.

Table 1a. Crystallographic Experimental Details for **4**•0.5C_7H_8.

A. Crystal Data	
formula	$C_{23.5}H_{30}BrMnNO_3P$
formula weight	540.31
crystal dimensions (mm)	$0.28 \times 0.16 \times 0.10$
crystal system	monoclinic
space group	$P2_1/c$ (No. 14)
unit cell parameters[a]	
a (Å)	15.5249 (11)
b (Å)	8.0752 (6)
c (Å)	20.4893 (14)
β (deg)	103.6339 (12)
V (Å^3)	2496.3 (3)
Z	4
ρ_{calcd} (g cm^{-3})	1.438
μ (mm^{-1})	2.217
B. Data Collection and Refinement Conditions	
diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.3°) (20 s exposures)
data collection 2θ limit (deg)	52.76
total data collected	16462 ($-19 \le h \le 19$, $-10 \le k \le 10$, $-25 \le l \le 25$)
independent reflections	5087 (R_{int} = 0.0458)
number of observed reflections (*NO*)	3851 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	Patterson search/structure expansion (*DIRDIF–99*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	multi-scan (*SADABS*)
range of transmission factors	0.8087–0.5757
data/restraints/parameters	5087 [$F_o^2 \ge -3\sigma(F_o^2)$] / 3[e] / 255
goodness-of-fit (S)[f]	1.033 [$F_o^2 \ge -3\sigma(F_o^2)$]
final R indices[g]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0521
wR_2 [$F_o^2 \ge -3\sigma(F_o^2)$]	0.1469
largest difference peak and hole	1.422 and –0.899 e Å^{-3}

[a]Obtained from least-squares refinement of 5071 reflections with $5.40° < 2\theta < 49.42°$.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table 1a. Crystallographic Experimental Details for **4**•0.5C_7H_8. (continued)

[c]Beurskens, P. T.; Beurskens, G.; de Gelder, R.; Garcia-Granda, S.; Israel, R.; Gould, R. O.; Smits, J. M. M. (1999). The *DIRDIF-99* program system. Crystallography Laboratory, University of Nijmegen, The Netherlands.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted *R*-factors wR_2 and all goodnesses of fit *S* are based on F_o^2; conventional *R*-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. *R*-factors based on F_o^2 are statistically about twice as large as those based on F_o, and *R*-factors based on ALL data will be even larger.

[e]Distances involving the methyl carbon of the inversion-disordered solvent toluene molecule were given fixed idealized values: d(C10S–C11S) = 1.54 Å; d(C10S···C12S) = d(C10S···C16S) = 2.54 Å. The aromatic ring of this molecule was refined as an idealized regular hexagon, with a fixed C–C bond length of 1.39 Å.

[f]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0789P)^2 + 3.3819P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[g]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2a. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for **4**•0.5C_7H_8.

(a) atoms of [{ κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}MnBr(CO)$_3$]

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Br	0.39818(3)	0.41748(6)	0.32246(2)	0.04154(16)*
Mn	0.27575(4)	0.23032(8)	0.26085(3)	0.03318(19)*
P	0.22891(7)	0.18758(13)	0.36035(5)	0.0279(2)*
O11	0.1311(4)	0.0550(6)	0.1736(2)	0.0823(14)*
O12	0.3492(3)	0.2698(6)	0.1412(2)	0.0794(13)*
O13	0.1729(3)	0.5336(5)	0.2212(2)	0.0722(12)*
N	0.3614(3)	0.0133(4)	0.29484(17)	0.0349(8)*
C1	0.4309(3)	-0.1442(6)	0.4062(2)	0.0401(10)*
C2	0.3648(3)	-0.0267(5)	0.3648(2)	0.0296(8)*
C3	0.3055(3)	0.0273(5)	0.39796(18)	0.0259(8)*
C3A	0.3222(3)	-0.0600(5)	0.46308(19)	0.0312(9)*
C4	0.2759(3)	-0.0586(6)	0.5133(2)	0.0420(11)*
C5	0.3074(4)	-0.1589(7)	0.5695(2)	0.0561(14)*
C6	0.3819(4)	-0.2529(7)	0.5755(3)	0.0612(16)*
C7	0.4270(4)	-0.2552(7)	0.5254(3)	0.0563(14)*
C7A	0.3964(3)	-0.1593(6)	0.4687(2)	0.0379(10)*
C11	0.1854(4)	0.1146(7)	0.2092(3)	0.0556(14)*
C12	0.3239(4)	0.2559(6)	0.1856(3)	0.0480(12)*
C13	0.2123(3)	0.4155(6)	0.2382(2)	0.0455(12)*
C21	0.1177(3)	0.1022(6)	0.3579(3)	0.0464(12)*
C22	0.1078(4)	-0.0759(7)	0.3334(3)	0.0639(16)*
C23	0.0453(3)	0.2121(9)	0.3153(4)	0.078(2)*
C24	0.2402(4)	0.3525(7)	0.4257(3)	0.0568(14)*
C25	0.2039(5)	0.5196(7)	0.3959(3)	0.0692(17)*
C26	0.3236(6)	0.3620(9)	0.4748(4)	0.100(3)*
C27	0.3230(4)	-0.1355(6)	0.2548(2)	0.0568(15)*
C28	0.4529(4)	0.0334(7)	0.2854(3)	0.0577(15)*

(b) solvent toluene atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C10S[a]	-0.0289(10)	0.2927(8)	0.4913(7)	0.0936(17)
C11S[a]	-0.0087(8)	0.1060(8)	0.4995(6)	0.0936(17)
C12S[a]	0.0545(7)	0.0489(10)	0.5547(5)	0.0936(17)
C13S[a]	0.0733(7)	-0.1193(10)	0.5618(5)	0.0936(17)
C14S[a]	0.0288(8)	-0.2305(8)	0.5137(6)	0.0936(17)
C15S[a]	-0.0344(7)	-0.1734(9)	0.4585(5)	0.0936(17)
C16S[a]	-0.0532(7)	-0.0051(10)	0.4514(5)	0.0936(17)

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$. [a]Atoms of the solvent toluene molecule were refined with an occupancy factor of 0.5 and a common isotropic displacement parameter.

Table 3a. Selected Interatomic Distances (Å) for **4**•0.5C_7H_8.

(a) within [{ κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}MnBr$(CO)_3$]

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Br	Mn	2.5218(8)	C1	C2	1.505(6)
Mn	P	2.3459(12)	C1	C7A	1.506(6)
Mn	N	2.211(4)	C2	C3	1.340(5)
Mn	C11	1.805(6)	C3	C3A	1.477(5)
Mn	C12	1.877(5)	C3A	C4	1.386(6)
Mn	C13	1.791(5)	C3A	C7A	1.386(6)
P	C3	1.803(4)	C4	C5	1.399(7)
P	C21	1.849(5)	C5	C6	1.363(8)
P	C24	1.866(5)	C6	C7	1.374(8)
O11	C11	1.089(6)	C7	C7A	1.383(6)
O12	C12	1.078(6)	C21	C22	1.519(8)
O13	C13	1.142(6)	C21	C23	1.533(7)
N	C2	1.457(5)	C24	C25	1.532(8)
N	C27	1.497(6)	C24	C26	1.444(9)
N	C28	1.488(6)			

(b) within the solvent toluene molecule

Atom1	Atom2	Distance	Atom1	Atom2	Distance
C10S	C11S	1.54†	C13S	C14S	1.39†
C11S	C12S	1.39†	C14S	C15S	1.39†
C11S	C16S	1.39†	C15S	C16S	1.39†
C12S	C13S	1.39†			

†Distance fixed during refinement.

Table 4a. Selected Interatomic Angles (deg) for **4**•0.5C_7H_8.

(a) within [{ κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}MnBr(CO)$_3$]

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
Br	Mn	P	90.26(3)	C2	C1	C7A	101.4(3)
Br	Mn	N	89.49(10)	N	C2	C1	123.8(3)
Br	Mn	C11	173.30(17)	N	C2	C3	123.9(4)
Br	Mn	C12	86.90(16)	C1	C2	C3	112.2(4)
Br	Mn	C13	86.17(16)	P	C3	C2	118.6(3)
P	Mn	N	84.04(9)	P	C3	C3A	133.3(3)
P	Mn	C11	94.39(18)	C2	C3	C3A	108.0(3)
P	Mn	C12	174.41(17)	C3	C3A	C4	131.0(4)
P	Mn	C13	94.81(17)	C3	C3A	C7A	108.5(4)
N	Mn	C11	95.8(2)	C4	C3A	C7A	120.6(4)
N	Mn	C12	91.12(19)	C3A	C4	C5	117.7(5)
N	Mn	C13	175.51(19)	C4	C5	C6	121.4(5)
C11	Mn	C12	88.9(2)	C5	C6	C7	120.7(5)
C11	Mn	C13	88.6(2)	C6	C7	C7A	119.0(5)
C12	Mn	C13	89.8(2)	C1	C7A	C3A	109.8(4)
Mn	P	C3	99.73(13)	C1	C7A	C7	129.6(5)
Mn	P	C21	120.64(17)	C3A	C7A	C7	120.6(5)
Mn	P	C24	121.5(2)	Mn	C11	O11	173.5(5)
C3	P	C21	105.2(2)	Mn	C12	O12	177.8(5)
C3	P	C24	105.4(2)	Mn	C13	O13	177.0(5)
C21	P	C24	102.4(3)	P	C21	C22	112.5(4)
Mn	N	C2	111.4(2)	P	C21	C23	110.7(4)
Mn	N	C27	109.3(3)	C22	C21	C23	110.9(5)
Mn	N	C28	113.2(3)	P	C24	C25	112.3(4)
C2	N	C27	106.2(3)	P	C24	C26	117.1(5)
C2	N	C28	109.7(4)	C25	C24	C26	114.6(6)
C27	N	C28	106.6(4)				

(b) within the solvent toluene molecule

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C10S	C11S	C12S	120.0†	C12S	C13S	C14S	120.0†
C10S	C11S	C16S	120.0†	C13S	C14S	C15S	120.0†
C12S	C11S	C16S	120.0†	C14S	C15S	C16S	120.0†
C11S	C12S	C13S	120.0†	C11S	C16S	C15S	120.0†

†Angle fixed during refinement.

Table 5a. Torsional Angles (deg) for **4**•0.5C_7H_8.

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
Br	Mn	P	C3	-82.56(13)	Br	Mn	C13	O13	96(9)
Br	Mn	P	C21	163.25(19)	P	Mn	C13	O13	-174(9)
Br	Mn	P	C24	32.3(2)	N	Mn	C13	O13	111(9)
N	Mn	P	C3	6.90(16)	C11	Mn	C13	O13	-80(9)
N	Mn	P	C21	-107.3(2)	C12	Mn	C13	O13	9(9)
N	Mn	P	C24	121.7(2)	Mn	P	C3	C2	-0.4(3)
C11	Mn	P	C3	102.3(2)	Mn	P	C3	C3A	176.1(4)
C11	Mn	P	C21	-11.9(3)	C21	P	C3	C2	125.2(4)
C11	Mn	P	C24	-142.9(3)	C21	P	C3	C3A	-58.3(4)
C12	Mn	P	C3	-23.2(17)	C24	P	C3	C2	-127.0(4)
C12	Mn	P	C21	-137.3(17)	C24	P	C3	C3A	49.4(5)
C12	Mn	P	C24	91.7(17)	Mn	P	C21	C22	66.7(4)
C13	Mn	P	C3	-168.7(2)	Mn	P	C21	C23	-58.1(5)
C13	Mn	P	C21	77.1(3)	C3	P	C21	C22	-44.7(4)
C13	Mn	P	C24	-53.9(3)	C3	P	C21	C23	-169.5(4)
Br	Mn	N	C2	77.3(3)	C24	P	C21	C22	-154.6(4)
Br	Mn	N	C27	-165.7(3)	C24	P	C21	C23	80.6(5)
Br	Mn	N	C28	-46.9(3)	Mn	P	C24	C25	49.4(5)
P	Mn	N	C2	-13.0(3)	Mn	P	C24	C26	-86.2(6)
P	Mn	N	C27	104.0(3)	C3	P	C24	C25	161.3(4)
P	Mn	N	C28	-137.3(3)	C3	P	C24	C26	25.7(6)
C11	Mn	N	C2	-106.9(3)	C21	P	C24	C25	-88.9(5)
C11	Mn	N	C27	10.2(3)	C21	P	C24	C26	135.5(6)
C11	Mn	N	C28	128.9(4)	Mn	N	C2	C1	-167.1(3)
C12	Mn	N	C2	164.2(3)	Mn	N	C2	C3	18.0(5)
C12	Mn	N	C27	-78.8(3)	C27	N	C2	C1	73.9(5)
C12	Mn	N	C28	40.0(4)	C27	N	C2	C3	-100.9(5)
C13	Mn	N	C2	62(2)	C28	N	C2	C1	-40.9(6)
C13	Mn	N	C27	179(100)	C28	N	C2	C3	144.2(4)
C13	Mn	N	C28	-62(2)	C7A	C1	C2	N	-171.7(4)
Br	Mn	C11	O11	10(7)	C7A	C1	C2	C3	3.6(5)
P	Mn	C11	O11	144(6)	C2	C1	C7A	C3A	-1.3(5)
N	Mn	C11	O11	-132(6)	C2	C1	C7A	C7	177.5(5)
C12	Mn	C11	O11	-40(6)	N	C2	C3	P	-11.8(6)
C13	Mn	C11	O11	49(6)	N	C2	C3	C3A	170.9(4)
Br	Mn	C12	O12	-152(14)	C1	C2	C3	P	172.8(3)
P	Mn	C12	O12	149(13)	C1	C2	C3	C3A	-4.5(5)
N	Mn	C12	O12	119(14)	P	C3	C3A	C4	8.8(7)
C11	Mn	C12	O12	23(14)	P	C3	C3A	C7A	-173.2(3)
C13	Mn	C12	O12	-65(14)	C2	C3	C3A	C4	-174.5(5)

Table 5a. Torsional Angles for **4**•0.5C_7H_8. (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C2	C3	C3A	C7A	3.5(5)	C6	C7	C7A	C1	-177.5(5)
C3	C3A	C4	C5	178.5(4)	C6	C7	C7A	C3A	1.2(8)
C7A	C3A	C4	C5	0.7(7)	C10S	C11S	C12S	C13S	-179.4(15)
C3	C3A	C7A	C1	-1.2(5)	C16S	C11S	C12S	C13S	0.0†
C3	C3A	C7A	C7	179.9(4)	C10S	C11S	C16S	C15S	179.4(15)
C4	C3A	C7A	C1	177.1(4)	C12S	C11S	C16S	C15S	0.0†
C4	C3A	C7A	C7	-1.8(7)	C11S	C12S	C13S	C14S	0.0†
C3A	C4	C5	C6	1.1(8)	C12S	C13S	C14S	C15S	0.0†
C4	C5	C6	C7	-1.8(9)	C13S	C14S	C15S	C16S	0.0†
C5	C6	C7	C7A	0.6(9)	C14S	C15S	C16S	C11S	0.0†

†Angle fixed during refinement.

Table 6a. Least-Squares Planes for **4**•0.5C_7H_8.

Plane	Coefficients[a]				Defining Atoms with Deviations (Å)[b]			
1	7.62(2)	6.123(8)	6.17(2)	4.918(10)				
					C1	-0.009(4)	C2	-0.049(3)
					C3	0.034(3)	C3A	0.029(4)
					C4	-0.006(4)	C5	-0.033(4)
					C6	-0.004(5)	C7	0.017(4)
					C7A	0.021(4)		
					P	0.200(5)	N	-0.262(5)

[a]Coefficients are for the form $ax+by+cz = d$ where x, y and z are crystallographic coordinates.
[b]Underlined atoms were not included in the definition of the plane.

Table 7a. Anisotropic Displacement Parameters (U_{ij}, Å^2) for **4**•0.5C_7H_8.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br	0.0411(3)	0.0352(3)	0.0496(3)	0.0024(2)	0.0134(2)	-0.00314(19)
Mn	0.0397(4)	0.0312(4)	0.0274(3)	0.0060(3)	0.0053(3)	-0.0018(3)
P	0.0276(5)	0.0253(5)	0.0310(5)	0.0034(4)	0.0070(4)	0.0017(4)
O11	0.097(3)	0.092(4)	0.043(2)	0.001(2)	-0.013(2)	-0.027(3)
O12	0.111(4)	0.090(3)	0.042(2)	0.007(2)	0.027(2)	-0.010(3)
O13	0.062(3)	0.057(3)	0.090(3)	0.030(2)	0.003(2)	0.018(2)
N	0.050(2)	0.0261(18)	0.0326(18)	-0.0017(15)	0.0184(16)	0.0043(16)
C1	0.039(2)	0.036(2)	0.045(3)	0.004(2)	0.009(2)	0.013(2)
C2	0.037(2)	0.023(2)	0.030(2)	0.0000(16)	0.0098(17)	0.0002(17)
C3	0.030(2)	0.0218(19)	0.0250(19)	0.0005(15)	0.0052(16)	-0.0014(16)
C3A	0.036(2)	0.030(2)	0.025(2)	0.0012(16)	0.0028(16)	-0.0025(18)
C4	0.051(3)	0.044(3)	0.032(2)	0.004(2)	0.011(2)	0.000(2)
C5	0.074(4)	0.062(3)	0.033(3)	0.012(2)	0.013(2)	-0.012(3)
C6	0.072(4)	0.061(4)	0.041(3)	0.025(3)	-0.005(3)	-0.003(3)
C7	0.054(3)	0.052(3)	0.056(3)	0.021(3)	-0.002(3)	0.009(3)
C7A	0.039(2)	0.035(2)	0.036(2)	0.0060(19)	0.0019(19)	0.001(2)
C11	0.062(3)	0.053(3)	0.047(3)	0.013(3)	0.005(3)	-0.013(3)
C12	0.060(3)	0.043(3)	0.041(3)	0.005(2)	0.012(2)	-0.007(2)
C13	0.042(3)	0.043(3)	0.048(3)	0.014(2)	0.003(2)	0.001(2)
C21	0.029(2)	0.055(3)	0.054(3)	0.016(2)	0.008(2)	-0.004(2)
C22	0.045(3)	0.063(4)	0.075(4)	0.016(3)	-0.004(3)	-0.023(3)
C23	0.028(3)	0.086(5)	0.115(6)	0.031(4)	0.003(3)	0.003(3)
C24	0.070(4)	0.042(3)	0.057(3)	-0.011(3)	0.014(3)	0.015(3)
C25	0.088(5)	0.038(3)	0.084(4)	-0.006(3)	0.026(3)	0.021(3)
C26	0.162(8)	0.062(4)	0.073(5)	-0.019(4)	0.019(5)	-0.012(5)
C27	0.106(5)	0.028(2)	0.038(3)	-0.010(2)	0.021(3)	0.000(3)
C28	0.064(3)	0.054(3)	0.069(4)	0.016(3)	0.045(3)	0.021(3)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table 8a. Derived Atomic Coordinates and Displacement Parameters for H-Atoms for **4**•0.5C_7H_8.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1A	0.4916	-0.0974	0.4162	0.048
H1B	0.4308	-0.2524	0.3835	0.048
H4	0.2246	0.0081	0.5096	0.050
H5	0.2763	-0.1616	0.6042	0.067
H6	0.4027	-0.3175	0.6148	0.073
H7	0.4786	-0.3217	0.5295	0.068
H21	0.1095	0.1034	0.4048	0.056
H22A	0.1567	-0.1424	0.3596	0.077
H22B	0.1090	-0.0797	0.2858	0.077
H22C	0.0513	-0.1206	0.3391	0.077
H23A	0.0540	0.3268	0.3311	0.094
H23B	-0.0130	0.1731	0.3193	0.094
H23C	0.0487	0.2068	0.2681	0.094
H24	0.1972	0.3180	0.4526	0.068
H25A	0.1464	0.5029	0.3643	0.083
H25B	0.2455	0.5690	0.3722	0.083
H25C	0.1966	0.5936	0.4321	0.083
H26A	0.3411	0.2511	0.4925	0.120
H26B	0.3173	0.4348	0.5117	0.120
H26C	0.3691	0.4067	0.4537	0.120
H27A	0.3181	-0.1141	0.2070	0.068
H27B	0.2640	-0.1585	0.2622	0.068
H27C	0.3616	-0.2312	0.2690	0.068
H28A	0.4504	0.0609	0.2384	0.069
H28B	0.4858	-0.0702	0.2972	0.069
H28C	0.4829	0.1227	0.3144	0.069
H10A[a]	-0.0120	0.3336	0.4510	0.112
H10B[a]	0.0049	0.3521	0.5308	0.112
H10C[a]	-0.0924	0.3112	0.4868	0.112
H12S[a]	0.0849	0.1249	0.5876	0.112
H13S[a]	0.1165	-0.1584	0.5996	0.112
H14S[a]	0.0416	-0.3455	0.5186	0.112
H15S[a]	-0.0648	-0.2493	0.4256	0.112
H16S[a]	-0.0964	0.0339	0.4137	0.112

[a]Included with an occupancy factor of 0.5.

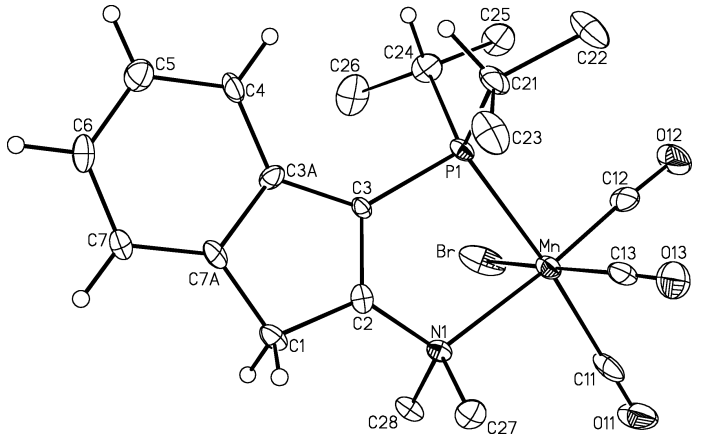

Figure 1aa. Perspective view of one of the two crystallographically independent $[(C_9H_6P\{^iPr\}_2N\{Me\}_2)(CO)_3MnBr]$ molecules (*molecule A*) showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 20% probability level. Hydrogen atoms are shown with arbitrarily small thermal parameters, and are not shown for the methyl groups.

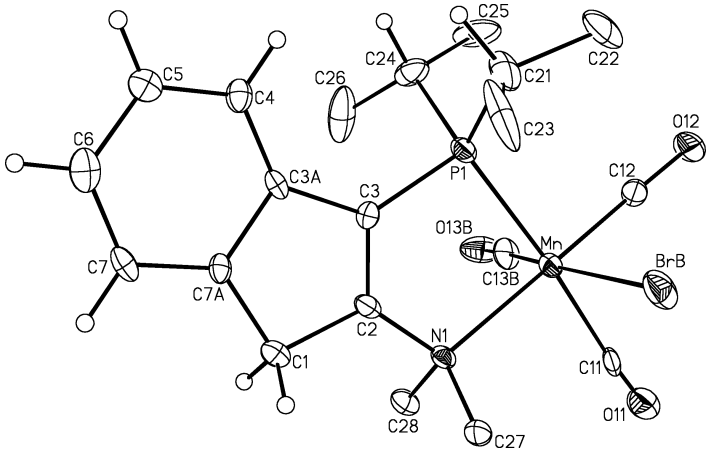

Figure 2aa. Perspective view of the second of two crystallographically independent $[(C_9H_6P\{^iPr\}_2N\{Me\}_2)(CO)_3MnBr]$ molecules (*molecule B*) showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 20% probability level. Only the major part (80%) of the bromide/carbonyl disorder (BrB, C13B and O13B) is shown for clarity. Hydrogen atoms are shown with arbitrarily small thermal parameters, and are not shown for the methyl groups.

Table 1aa. Crystallographic Experimental Details for **4**•0.5C_7H_8.

A. Crystal Data	
formula	$C_{23.50}H_{30}BrMnNO_3P$
formula weight	540.31
crystal dimensions (mm)	0.20 x 0.10 x 0.05
crystal system	monoclinic
space group	$P2_1$ (No. 4)
unit cell parameters[a]	
a (Å)	8.3609 (7)
b (Å)	29.333 (2)
c (Å)	10.0818 (8)
β (deg)	99.222 (2)
V (Å^3)	2440.6 (3)
Z	4
ρ_{calcd} (g cm^{-3})	1.470
μ (mm^{-1})	2.268
B. Data Collection and Refinement Conditions	
diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.2°) (25 s exposures)
data collection 2θ limit (deg)	50.00
total data collected	15191 ($-9 \le h \le 9$, $-32 \le k \le 34$, $-11 \le l \le 11$)
independent reflections	8364 (R_{int} = 0.0639)
number of observed reflections (*NO*)	5109 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–86*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	multi-scan (*SADABS*)
range of transmission factors	0.8951–0.6598
data/restraints/parameters	8364 [$F_o^2 \ge -3\sigma(F_o^2)$] / 7[e] / 531
Flack absolute structure parameter[f]	0.217(17)
goodness-of-fit (S)[g]	1.002 [$F_o^2 \ge -3\sigma(F_o^2)$]
final R indices[h]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0664
wR_2 [$F_o^2 \ge -3\sigma(F_o^2)$]	0.1513
largest difference peak and hole	0.458 and –0.498 e Å^{-3}

[a]Obtained from least-squares refinement of 2016 reflections with 4.32° < 2θ < 42.83°.

(continued)

Table 1aa. Crystallographic Experimental Details for **4**•0.5C_7H_8. (continued)

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

[c]Sheldrick, G. M. *Acta Crystallogr.* **1990**, *A46*, 467–473.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted *R*-factors wR_2 and all goodnesses of fit *S* are based on F_o^2; conventional *R*-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. *R*-factors based on F_o^2 are statistically about twice as large as those based on F_o, and *R*-factors based on ALL data will be even larger.

[e]The C13C–O13C distance was restrained to be 1.15(1) Å. The C50–C51 and C60–C61 distances were restrained to be 1.54(1) Å. The C50···C52, C50···C56, C60···C62 and C60···C66 distances were restrained to be 2.54(1) Å. The solvent toluene rings were constrained to be idealized hexagons with C–C distances of 1.39 Å.

[f]Flack, H. D. *Acta Crystallogr.* **1983**, *A39*, 876–881; Flack, H. D.; Bernardinelli, G. *Acta Crystallogr.* **1999**, *A55*, 908–915; Flack, H. D.; Bernardinelli, G. *J. Appl. Cryst.* **2000**, *33*, 1143–1148. The Flack parameter will refine to a value near zero if the structure is in the correct configuration and will refine to a value near one for the inverted configuration. The value observed herein is indicative of racemic twinning, and was accomodated during the refinement (using the *SHELXL-93* TWIN instruction [see reference *d*]).

[g]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0638P)^2]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[h]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2aa. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for **4**•0.5C_7H_8.

(a) atoms of molecule A

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Br	-0.49299(14)	0.19819(6)	0.29839(17)	0.0833(5)*
Mn	-0.30355(16)	0.25496(7)	0.21703(13)	0.0356(4)*
P1	-0.2466(3)	0.28809(10)	0.4293(2)	0.0291(6)*
O11	-0.3575(10)	0.2070(4)	-0.0380(9)	0.090(3)*
O12	-0.5991(10)	0.3080(3)	0.1355(8)	0.079(3)*
O13	-0.1344(13)	0.3221(3)	0.0795(9)	0.078(3)*
N1	-0.0882(8)	0.2122(2)	0.2906(7)	0.0275(18)*
C1	0.1204(10)	0.1972(4)	0.5086(9)	0.037(2)*
C2	-0.0237(10)	0.2202(3)	0.4316(8)	0.028(2)*
C3	-0.0839(9)	0.2519(3)	0.5069(8)	0.0238(19)*
C3A	0.0148(10)	0.2511(4)	0.6400(8)	0.034(2)*
C4	0.0008(11)	0.2758(4)	0.7582(9)	0.042(3)*
C5	0.1084(13)	0.2671(4)	0.8756(9)	0.049(3)*
C6	0.2260(12)	0.2341(4)	0.8753(10)	0.045(3)*
C7	0.2411(11)	0.2088(3)	0.7611(9)	0.036(2)*
C7A	0.1359(11)	0.2176(3)	0.6446(9)	0.031(2)*
C11	-0.3352(13)	0.2238(4)	0.0473(13)	0.055(3)*
C12	-0.4845(13)	0.2873(4)	0.1702(9)	0.052(3)*
C13	-0.1858(16)	0.2993(5)	0.1349(12)	0.058(4)*
C21	-0.1539(13)	0.3452(3)	0.4455(10)	0.047(3)*
C22	-0.2677(14)	0.3820(4)	0.3710(12)	0.071(4)*
C23	0.0155(14)	0.3478(4)	0.4095(12)	0.060(3)*
C24	-0.3928(11)	0.2904(4)	0.5472(9)	0.049(3)*
C25	-0.5638(12)	0.3053(5)	0.4793(11)	0.068(4)*
C26	-0.4032(13)	0.2464(5)	0.6284(11)	0.074(4)*
C27	0.0438(11)	0.2214(4)	0.2089(9)	0.041(3)*
C28	-0.1255(12)	0.1626(3)	0.2742(10)	0.042(3)*

(b) atoms of molecule B

Atom	*x*	*y*	*z*	U_{eq}, Å^2
BrB	-0.52090(17)	0.09969(8)	-0.27157(19)	0.0687(5)*[a]
BrC	-0.1182(18)	-0.0158(5)	-0.3790(12)	0.071(3)[b]
Mn	-0.30822(17)	0.04235(7)	-0.31439(13)	0.0347(4)*
P1	-0.2628(3)	0.01423(11)	-0.0961(2)	0.0373(7)*
O11	-0.3476(10)	0.0785(3)	-0.5821(9)	0.074(3)*
O12	-0.5931(10)	-0.0156(3)	-0.3984(8)	0.067(2)*
O13B	-0.114(2)	-0.0251(5)	-0.4252(17)	0.076(5)*[a]
O13C	-0.488(4)	0.1022(11)	-0.185(3)	0.034(7)[b,c]
N1	-0.1041(9)	0.0891(3)	-0.2395(6)	0.0319(19)*

Table 2aa. Atomic Coordinates and Displacement Parameters for **4**•0.5C_7H_8. (continued)

(b) atoms of molecule B

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C1	0.1086(12)	0.1056(4)	-0.0209(9)	0.043(3)*
C2	-0.0375(11)	0.0799(3)	-0.0983(9)	0.035(2)*
C3	-0.0963(10)	0.0494(3)	-0.0231(8)	0.029(2)*
C3A	-0.0012(10)	0.0504(3)	0.1144(8)	0.025(2)*
C4	-0.0109(11)	0.0265(4)	0.2286(8)	0.040(3)*
C5	0.0936(12)	0.0350(4)	0.3435(10)	0.045(3)*
C6	0.2142(13)	0.0681(4)	0.3466(11)	0.054(3)*
C7	0.2263(11)	0.0937(4)	0.2331(10)	0.041(3)*
C7A	0.1199(10)	0.0841(3)	0.1162(9)	0.032(2)*
C11	-0.3324(11)	0.0694(4)	-0.4877(11)	0.042(3)*
C12	-0.4784(13)	0.0066(3)	-0.3659(10)	0.042(3)*
C13B	-0.1944(18)	0.0031(6)	-0.3723(16)	0.056(5)*[a]
C13C	-0.440(5)	0.0793(13)	-0.263(4)	0.034(7)[b,c]
C21	-0.4148(14)	0.0211(6)	0.0199(11)	0.080(5)*
C22	-0.5798(15)	0.0041(6)	-0.0439(14)	0.093(5)*
C23	-0.4219(14)	0.0670(6)	0.0738(13)	0.116(7)*
C24	-0.1886(16)	-0.0447(4)	-0.0642(11)	0.063(4)*
C25	-0.2951(19)	-0.0799(4)	-0.1476(12)	0.095(5)*
C26	-0.0154(18)	-0.0503(5)	-0.0836(15)	0.108(7)*
C27	-0.1515(12)	0.1381(3)	-0.2523(10)	0.047(3)*
C28	0.0303(12)	0.0823(4)	-0.3198(9)	0.045(3)*

(c) solvent toluene atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C50	0.7319(17)	0.4324(8)	0.739(3)	0.120(9)[d]
C51	0.5640(14)	0.4125(5)	0.7504(16)	0.094(7)[d]
C52	0.5517(17)	0.3738(5)	0.8279(16)	0.072(6)[d]
C53	0.400(2)	0.3558(6)	0.8375(18)	0.140(12)[d]
C54	0.2611(16)	0.3764(6)	0.7698(17)	0.091(7)[d]
C55	0.2734(15)	0.4151(6)	0.6923(17)	0.107(8)[d]
C56	0.4248(17)	0.4331(5)	0.6826(17)	0.11(2)[d]
C60	0.1815(17)	0.3960(10)	0.720(3)	0.102(11)[e]
C61	0.3674(16)	0.4010(6)	0.7465(18)	0.053(6)[e]
C62	0.462(2)	0.3683(6)	0.822(2)	0.057(7)[e]
C63	0.630(2)	0.3718(8)	0.841(2)	0.107(13)[e]
C64	0.7032(17)	0.4081(9)	0.785(2)	0.096(11)[e]
C65	0.608(2)	0.4408(8)	0.710(2)	0.093(11)[e]
C66	0.440(2)	0.4372(7)	0.691(2)	0.07(2)[e]

Table 2aa. Atomic Coordinates and Displacement Parameters for **4**•0.5C_7H_8. (continued)

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$. [a]Refined with an occupancy factor of 0.8. [b]Refined with an occupancy factor of 0.2. [c]Refined with a common isotropic displacement parameter. [d]Refined with an occupancy factor of 0.6. [e]Refined with an occupancy factor of 0.4.

Table 3aa. Selected Interatomic Distances (Å) for **4**•0.5C_7H_8.

(a) within molecule A

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Br	Mn	2.524(2)	C1	C2	1.488(11)
Mn	P1	2.329(3)	C1	C7A	1.483(12)
Mn	N1	2.222(7)	C2	C3	1.348(12)
Mn	C11	1.920(13)	C3	C3A	1.458(10)
Mn	C12	1.784(11)	C3A	C4	1.415(13)
Mn	C13	1.899(16)	C3A	C7A	1.406(13)
P1	C3	1.802(8)	C4	C5	1.391(12)
P1	C21	1.842(10)	C5	C6	1.379(14)
P1	C24	1.838(10)	C6	C7	1.391(14)
O11	C11	0.983(11)	C7	C7A	1.375(12)
O12	C12	1.142(12)	C21	C22	1.552(13)
O13	C13	1.012(15)	C21	C23	1.519(15)
N1	C2	1.456(10)	C24	C25	1.546(12)
N1	C27	1.503(12)	C24	C26	1.538(15)
N1	C28	1.491(12)			

(b) within molecule B

Atom1	Atom2	Distance	Atom1	Atom2	Distance
BrB	Mn	2.534(2)	N1	C27	1.491(12)
BrC	Mn	2.489(16)	N1	C28	1.500(12)
Mn	P1	2.324(3)	C1	C2	1.539(12)
Mn	N1	2.226(7)	C1	C7A	1.508(13)
Mn	C11	1.900(11)	C2	C3	1.316(12)
Mn	C12	1.777(11)	C3	C3A	1.484(11)
Mn	C13B	1.658(16)	C3A	C4	1.360(13)
Mn	C13C	1.69(3)	C3A	C7A	1.414(12)
P1	C3	1.794(9)	C4	C5	1.357(12)
P1	C21	1.871(12)	C5	C6	1.398(15)
P1	C24	1.846(12)	C6	C7	1.386(15)
O11	C11	0.977(10)	C7	C7A	1.387(12)
O12	C12	1.161(11)	C21	C22	1.511(15)
O13B	C13B	1.24(2)	C21	C23	1.46(2)
O13C	C13C	1.15(1)†	C24	C25	1.525(15)
N1	C2	1.468(11)	C24	C26	1.50(2)

†Distance restrained during refinement.

Table 3aa. Selected Interatomic Distances for **4**•0.5C_7H_8. (continued)

(c) within the solvent toluene molecules

Atom1	Atom2	Distance	Atom1	Atom2	Distance
C50	C51	1.54(1)[a]	C60	C61	1.54(1)[a]
C51	C52	1.39[b]	C61	C62	1.39[b]
C51	C56	1.39[b]	C61	C66	1.39[b]
C52	C53	1.39[b]	C62	C63	1.39[b]
C53	C54	1.39[b]	C63	C64	1.39[b]
C54	C55	1.39[b]	C64	C65	1.39[b]
C55	C56	1.39[b]	C65	C66	1.39[b]

[a]Distance restrained during refinement. [b]Distance constrained during refinement.

Table 4aa. Selected Interatomic Angles (deg) for **4**•0.5C_7H_8.

(a) within molecule A

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
Br	Mn	P1	91.33(9)	C2	C1	C7A	104.0(8)
Br	Mn	N1	92.1(2)	N1	C2	C1	125.3(8)
Br	Mn	C11	88.4(4)	N1	C2	C3	123.2(7)
Br	Mn	C12	83.5(4)	C1	C2	C3	111.3(7)
Br	Mn	C13	171.7(3)	P1	C3	C2	119.1(6)
P1	Mn	N1	83.87(19)	P1	C3	C3A	133.3(7)
P1	Mn	C11	174.9(3)	C2	C3	C3A	107.4(7)
P1	Mn	C12	93.5(3)	C3	C3A	C4	131.0(8)
P1	Mn	C13	94.1(3)	C3	C3A	C7A	109.9(8)
N1	Mn	C11	91.0(3)	C4	C3A	C7A	119.0(7)
N1	Mn	C12	174.8(4)	C3A	C4	C5	119.6(10)
N1	Mn	C13	94.8(4)	C4	C5	C6	119.4(10)
C11	Mn	C12	91.6(4)	C5	C6	C7	122.3(8)
C11	Mn	C13	86.8(5)	C6	C7	C7A	118.4(9)
C12	Mn	C13	89.9(5)	C1	C7A	C3A	107.3(7)
Mn	P1	C3	100.5(3)	C1	C7A	C7	131.5(9)
Mn	P1	C21	118.8(3)	C3A	C7A	C7	121.2(9)
Mn	P1	C24	123.4(3)	Mn	C11	O11	176.4(14)
C3	P1	C21	102.7(4)	Mn	C12	O12	177.4(10)
C3	P1	C24	105.9(4)	Mn	C13	O13	172.1(13)
C21	P1	C24	102.9(5)	P1	C21	C22	112.0(7)
Mn	N1	C2	112.8(5)	P1	C21	C23	114.8(7)
Mn	N1	C27	110.0(5)	C22	C21	C23	111.8(9)
Mn	N1	C28	111.7(5)	P1	C24	C25	112.8(7)
C2	N1	C27	108.5(6)	P1	C24	C26	114.5(8)
C2	N1	C28	107.7(7)	C25	C24	C26	110.3(9)
C27	N1	C28	105.9(7)				

(b) within molecule B

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
BrB	Mn	P1	94.99(9)	BrC	Mn	C13C	176.2(15)
BrB	Mn	N1	93.1(2)	P1	Mn	N1	84.11(19)
BrB	Mn	C11	84.5(3)	P1	Mn	C11	175.0(3)
BrB	Mn	C12	83.7(3)	P1	Mn	C12	93.9(3)
BrB	Mn	C13B	168.1(5)	P1	Mn	C13B	94.1(5)
BrC	Mn	P1	89.4(3)	P1	Mn	C13C	87.2(15)
BrC	Mn	N1	91.4(3)	N1	Mn	C11	91.0(4)
BrC	Mn	C11	91.4(5)	N1	Mn	C12	176.1(4)
BrC	Mn	C12	91.9(5)	N1	Mn	C13B	95.5(6)

Table 4aa. Selected Interatomic Angles for **4**•0.5C_7H_8. (continued)

(b) within molecule B

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
N1	Mn	C13C	90.1(15)	P1	C3	C3A	131.2(7)
C11	Mn	C12	90.9(4)	C2	C3	C3A	109.4(8)
C11	Mn	C13B	87.1(6)	C3	C3A	C4	133.3(8)
C11	Mn	C13C	92.1(15)	C3	C3A	C7A	107.4(8)
C12	Mn	C13B	88.0(6)	C4	C3A	C7A	119.3(8)
C12	Mn	C13C	86.5(15)	C3A	C4	C5	120.7(10)
Mn	P1	C3	100.5(3)	C4	C5	C6	120.6(10)
Mn	P1	C21	121.9(4)	C5	C6	C7	120.4(9)
Mn	P1	C24	119.8(4)	C6	C7	C7A	118.1(10)
C3	P1	C21	104.0(5)	C1	C7A	C3A	110.0(7)
C3	P1	C24	104.5(5)	C1	C7A	C7	129.2(9)
C21	P1	C24	103.6(7)	C3A	C7A	C7	120.8(9)
Mn	N1	C2	111.5(5)	Mn	C11	O11	171.1(12)
Mn	N1	C27	112.7(5)	Mn	C12	O12	177.6(10)
Mn	N1	C28	109.5(5)	Mn	C13B	O13B	175.2(17)
C2	N1	C27	108.5(7)	Mn	C13C	O13C	154(4)
C2	N1	C28	107.4(6)	P1	C21	C22	111.3(9)
C27	N1	C28	107.1(7)	P1	C21	C23	113.9(10)
C2	C1	C7A	100.8(8)	C22	C21	C23	112.0(12)
N1	C2	C1	123.2(8)	P1	C24	C25	112.8(8)
N1	C2	C3	124.4(8)	P1	C24	C26	112.6(9)
C1	C2	C3	112.3(8)	C25	C24	C26	110.1(12)
P1	C3	C2	119.4(6)				

(c) within the solvent toluene molecules

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C50	C51	C52	120.0(1)[a]	C60	C61	C62	120.0(1)[a]
C50	C51	C56	120.0(1)[a]	C60	C61	C66	120.0(1)[a]
C52	C51	C56	120.0[b]	C62	C61	C66	120.0[b]
C51	C52	C53	120.0[b]	C61	C62	C63	120.0[b]
C52	C53	C54	120.0[b]	C62	C63	C64	120.0[b]
C53	C54	C55	120.0[b]	C63	C64	C65	120.0[b]
C54	C55	C56	120.0[b]	C64	C65	C66	120.0[b]
C51	C56	C55	120.0[b]	C61	C66	C65	120.0[b]

[a]Angle restrained during refinement. [b]Angle constrained during refinement.

Table 5aa. Torsional Angles (deg) for **4**•0.5C_7H_8.

(a) within molecule A

Atom1	Atom2	Atom3	Atom4	Angle
Br	Mn	P1	C3	86.2(3)
Br	Mn	P1	C21	-162.9(4)
Br	Mn	P1	C24	-30.9(4)
N1	Mn	P1	C3	-5.7(3)
N1	Mn	P1	C21	105.2(4)
N1	Mn	P1	C24	-122.9(5)
C11	Mn	P1	C3	0(5)
C11	Mn	P1	C21	110(5)
C11	Mn	P1	C24	-118(5)
C12	Mn	P1	C3	169.8(5)
C12	Mn	P1	C21	-79.3(6)
C12	Mn	P1	C24	52.7(6)
C13	Mn	P1	C3	-100.1(4)
C13	Mn	P1	C21	10.8(5)
C13	Mn	P1	C24	142.8(5)
Br	Mn	N1	C2	-85.5(5)
Br	Mn	N1	C27	153.2(5)
Br	Mn	N1	C28	36.0(6)
P1	Mn	N1	C2	5.6(5)
P1	Mn	N1	C27	-115.7(5)
P1	Mn	N1	C28	127.1(6)
C11	Mn	N1	C2	-174.0(6)
C11	Mn	N1	C27	64.8(7)
C11	Mn	N1	C28	-52.5(7)
C12	Mn	N1	C2	-54(4)
C12	Mn	N1	C27	-175(4)
C12	Mn	N1	C28	67(4)
C13	Mn	N1	C2	99.2(6)
C13	Mn	N1	C27	-22.1(6)
C13	Mn	N1	C28	-139.3(7)
Br	Mn	C11	O11	17(18)
P1	Mn	C11	O11	104(17)
N1	Mn	C11	O11	109(18)
C12	Mn	C11	O11	-66(18)
C13	Mn	C11	O11	-156(18)
Br	Mn	C12	O12	-124(24)
P1	Mn	C12	O12	145(24)
N1	Mn	C12	O12	-156(21)
C11	Mn	C12	O12	-36(24)
C13	Mn	C12	O12	51(24)
Br	Mn	C13	O13	-18(11)
P1	Mn	C13	O13	-149(9)
N1	Mn	C13	O13	127(9)
C11	Mn	C13	O13	37(9)
C12	Mn	C13	O13	-55(9)
Mn	P1	C3	C2	6.4(8)
Mn	P1	C3	C3A	-179.8(8)
C21	P1	C3	C2	-116.6(8)
C21	P1	C3	C3A	57.2(10)
C24	P1	C3	C2	135.8(8)
C24	P1	C3	C3A	-50.4(10)
Mn	P1	C21	C22	64.2(9)
Mn	P1	C21	C23	-64.7(8)
C3	P1	C21	C22	173.9(8)
C3	P1	C21	C23	45.0(8)
C24	P1	C21	C22	-76.2(9)
C24	P1	C21	C23	154.9(7)
Mn	P1	C24	C25	-45.5(11)
Mn	P1	C24	C26	81.7(8)
C3	P1	C24	C25	-160.0(9)
C3	P1	C24	C26	-32.8(9)
C21	P1	C24	C25	92.6(9)
C21	P1	C24	C26	-140.2(8)
Mn	N1	C2	C1A	-179.3(7)
Mn	N1	C2	C3	-3.2(10)
C27	N1	C2	C1	-57.2(10)
C27	N1	C2	C3	118.9(9)
C28	N1	C2	C1	57.0(11)
C28	N1	C2	C3	-126.9(9)
C7A	C1	C2	N1	179.2(7)
C7A	C1	C2	C3	2.7(10)
C2	C1	C7A	C3A	-3.0(10)
C2	C1	C7A	C7	176.7(9)
N1	C2	C3	P1	-2.6(12)
N1	C2	C3	C3A	-177.9(7)
C1	C2	C3	P1	173.9(6)
C1	C2	C3	C3A	-1.3(10)
P1	C3	C3A	C4	8.7(17)

Table 5aa. Torsional Angles for **4**•0.5C_7H_8. (continued)

(a) within molecule A

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
P1	C3	C3A	C7A	-175.0(7)	C4	C3A	C7A	C1	179.2(9)
C2	C3	C3A	C4	-177.0(10)	C4	C3A	C7A	C7	-0.6(14)
C2	C3	C3A	C7A	-0.7(11)	C3A	C4	C5	C6	-0.8(16)
C3	C3A	C4	C5	177.2(10)	C4	C5	C6	C7	-0.1(16)
C7A	C3A	C4	C5	1.1(15)	C5	C6	C7	C7A	0.7(15)
C3	C3A	C7A	C1	2.4(10)	C6	C7	C7A	C1	180.0(9)
C3	C3A	C7A	C7	-177.4(8)	C6	C7	C7A	C3A	-0.4(14)

(b) within molecule b

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
BrB	Mn	P1	C3	-93.0(3)	P1	Mn	N1	C28	120.5(5)
BrB	Mn	P1	C21	20.9(6)	C11	Mn	N1	C2	-178.9(6)
BrB	Mn	P1	C24	153.4(5)	C11	Mn	N1	C27	58.9(7)
BrC	Mn	P1	C3	91.0(4)	C11	Mn	N1	C28	-60.2(6)
BrC	Mn	P1	C21	-155.1(6)	C12	Mn	N1	C2	61(6)
BrC	Mn	P1	C24	-22.5(6)	C12	Mn	N1	C27	-61(6)
N1	Mn	P1	C3	-0.4(4)	C12	Mn	N1	C28	-180(100)
N1	Mn	P1	C21	113.5(6)	C13B	Mn	N1	C2	-91.7(8)
N1	Mn	P1	C24	-114.0(5)	C13B	Mn	N1	C27	146.0(8)
C11	Mn	P1	C3	-9(4)	C13B	Mn	N1	C28	27.0(8)
C11	Mn	P1	C21	105(4)	C13C	Mn	N1	C2	89.0(16)
C11	Mn	P1	C24	-122(4)	C13C	Mn	N1	C27	-33.3(16)
C12	Mn	P1	C3	-177.1(5)	C13C	Mn	N1	C28	-152.3(16)
C12	Mn	P1	C21	-63.2(7)	BrB	Mn	C11	O11	-127(7)
C12	Mn	P1	C24	69.4(6)	BrC	Mn	C11	O11	48(7)
C13B	Mn	P1	C3	94.7(6)	P1	Mn	C11	O11	148(5)
C13B	Mn	P1	C21	-151.4(8)	N1	Mn	C11	O11	140(7)
C13B	Mn	P1	C24	-18.9(7)	C12	Mn	C11	O11	-44(7)
C13C	Mn	P1	C3	-90.8(15)	C13B	Mn	C11	O11	44(7)
C13C	Mn	P1	C21	23.1(16)	C13C	Mn	C11	O11	-130(7)
C13C	Mn	P1	C24	155.7(16)	BrB	Mn	C12	O12	-1(23)
BrB	Mn	N1	C2	96.5(6)	BrC	Mn	C12	O12	-177(100)
BrB	Mn	N1	C27	-25.7(6)	P1	Mn	C12	O12	94(23)
BrB	Mn	N1	C28	-144.8(5)	N1	Mn	C12	O12	35(26)
BrC	Mn	N1	C2	-87.5(6)	C11	Mn	C12	O12	-85(23)
BrC	Mn	N1	C27	150.3(7)	C13B	Mn	C12	O12	-172(23)
BrC	Mn	N1	C28	31.2(6)	C13C	Mn	C12	O12	7(23)
P1	Mn	N1	C2	1.8(5)	BrB	Mn	C13B	O13B	28(19)
P1	Mn	N1	C27	-120.4(6)	P1	Mn	C13B	O13B	168(17)

Table 5aa. Torsional Angles for **4**•0.5C_7H_8. (continued)

(b) within molecule B

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
N1	Mn	C13B	O13B	-108(17)	Mn	N1	C2	C3	-3.4(11)
C11	Mn	C13B	O13B	-17(17)	C27	N1	C2	C1	-57.7(11)
C12	Mn	C13B	O13B	74(17)	C27	N1	C2	C3	121.3(10)
C13C	Mn	C13B	O13B	65(25)	C28	N1	C2	C1	57.7(11)
BrC	Mn	C13C	O13C	60(28)	C28	N1	C2	C3	-123.4(10)
P1	Mn	C13C	O13C	31(9)	C7A	C1	C2	N1	178.1(8)
N1	Mn	C13C	O13C	-54(9)	C7A	C1	C2	C3	-1.0(11)
C11	Mn	C13C	O13C	-145(9)	C2	C1	C7A	C3A	1.0(10)
C12	Mn	C13C	O13C	125(9)	C2	C1	C7A	C7	-178.2(9)
C13B	Mn	C13C	O13C	134(13)	N1	C2	C3	P1	3.2(13)
Mn	P1	C3	C2	-1.2(8)	N1	C2	C3	C3A	-178.5(8)
Mn	P1	C3	C3A	-179.1(8)	C1	C2	C3	P1	-177.8(7)
C21	P1	C3	C2	-128.1(9)	C1	C2	C3	C3A	0.5(11)
C21	P1	C3	C3A	54.0(10)	P1	C3	C3A	C4	-2.1(15)
C24	P1	C3	C2	123.5(9)	P1	C3	C3A	C7A	178.2(7)
C24	P1	C3	C3A	-54.4(9)	C2	C3	C3A	C4	179.9(10)
Mn	P1	C21	C22	52.8(13)	C2	C3	C3A	C7A	0.2(10)
Mn	P1	C21	C23	-75.1(10)	C3	C3A	C4	C5	-179.4(9)
C3	P1	C21	C22	164.9(10)	C7A	C3A	C4	C5	0.3(14)
C3	P1	C21	C23	37.1(10)	C3	C3A	C7A	C1	-0.8(10)
C24	P1	C21	C22	-86.1(11)	C3	C3A	C7A	C7	178.5(8)
C24	P1	C21	C23	146.1(9)	C4	C3A	C7A	C1	179.5(8)
Mn	P1	C24	C25	-54.3(11)	C4	C3A	C7A	C7	-1.2(13)
Mn	P1	C24	C26	71.0(9)	C3A	C4	C5	C6	-0.4(15)
C3	P1	C24	C25	-165.7(9)	C4	C5	C6	C7	1.5(15)
C3	P1	C24	C26	-40.4(9)	C5	C6	C7	C7A	-2.4(15)
C21	P1	C24	C25	85.6(10)	C6	C7	C7A	C1	-178.6(9)
C21	P1	C24	C26	-149.0(9)	C6	C7	C7A	C3A	2.2(14)
Mn	N1	C2	C1	177.7(7)					

Table 5aa. Torsional Angles for **4**•0.5C_7H_8. (continued)

(c) within solvent toluene molecules

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C50	C51	C52	C53	-179.8(19)	C60	C61	C62	C63	178(2)
C56	C51	C52	C53	0.0	C66	C61	C62	C63	0.0
C50	C51	C56	C55	179.8(19)	C60	C61	C66	C65	-178(2)
C52	C51	C56	C55	0.0	C62	C61	C66	C65	0.0
C51	C52	C53	C54	0.0	C61	C62	C63	C64	0.0
C52	C53	C54	C55	0.0	C62	C63	C64	C65	0.0
C53	C54	C55	C56	0.0	C63	C64	C65	C66	0.0
C54	C55	C56	C51	0.0	C64	C65	C66	C61	0.0

Table 6aa. Least-Squares Planes for **4**•0.5C_7H_8.

Plane	Coefficients[a]			Defining Atoms with Deviations (Å)[b]			
1	5.62(2)	20.26(7)	-3.752(19)	2.74(2)			
				C1	0.022(7)	C2	-0.031(7)
				C3	-0.009(7)	C3A	0.029(9)
				C4	0.006(8)	C5	-0.006(8)
				C6	-0.013(8)	C7	-0.011(7)
				C7A	0.013(8)		
				<u>P1</u>	0.101(11)	<u>N1</u>	-0.027(11)
				<u>Mn</u>	-0.094(12)		
2	-5.67(2)	20.13(6)	3.71(2)	1.448(6)			
				C1	-0.016(8)	C2	0.007(8)
				C3	0.007(7)	C3A	-0.002(7)
				C4	-0.004(8)	C5	-0.001(8)
				C6	-0.005(8)	C7	0.019(8)
				C7A	-0.004(8)		
				<u>P1</u>	-0.029(11)	<u>N1</u>	0.047(11)
				<u>Mn</u>	-0.015(12)		

Note: plane 1 refers to molecule A; plane 2 refers to molecule B.

[a]Coefficients are for the form $ax+by+cz = d$ where x, y and z are crystallographic coordinates.

[b]Underlined atoms were not included in the definition of the plane.

Table 7aa. Anisotropic Displacement Parameters (U_{ij}, Å^2) for **4**•0.5C_7H_8.

(a) within molecule A

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br	0.0426(7)	0.0533(8)	0.1596(13)	-0.0243(9)	0.0332(8)	-0.0081(6)
Mn	0.0309(8)	0.0313(8)	0.0423(8)	-0.0042(7)	-0.0010(6)	0.0068(7)
P1	0.0208(12)	0.0248(13)	0.0407(13)	-0.0003(11)	0.0025(10)	0.0061(10)
O11	0.074(6)	0.107(8)	0.079(6)	-0.043(6)	-0.020(5)	0.048(6)
O12	0.067(6)	0.079(6)	0.079(5)	-0.018(4)	-0.028(5)	0.039(5)
O13	0.115(8)	0.058(7)	0.072(6)	0.025(5)	0.047(5)	0.012(6)
N1	0.027(4)	0.019(4)	0.037(4)	-0.003(3)	0.007(3)	-0.004(3)
C1	0.028(5)	0.034(6)	0.052(6)	0.008(5)	0.014(4)	0.010(5)
C2	0.022(5)	0.025(5)	0.036(5)	0.010(4)	0.002(4)	-0.012(4)
C3	0.019(4)	0.024(5)	0.028(4)	0.004(4)	0.004(3)	0.007(4)
C3A	0.026(5)	0.052(6)	0.024(4)	-0.005(5)	0.008(4)	0.003(5)
C4	0.036(7)	0.045(7)	0.043(6)	0.011(5)	0.000(5)	0.019(5)
C5	0.047(7)	0.056(8)	0.043(6)	-0.003(5)	0.001(5)	-0.002(6)
C6	0.033(6)	0.058(7)	0.041(6)	0.013(5)	-0.010(5)	-0.004(5)
C7	0.031(5)	0.036(6)	0.039(6)	0.011(5)	0.002(4)	0.006(5)
C7A	0.032(5)	0.019(5)	0.044(6)	0.018(4)	0.012(4)	0.002(4)
C11	0.035(6)	0.044(7)	0.076(9)	-0.012(6)	-0.023(6)	0.021(5)
C12	0.048(7)	0.063(8)	0.038(6)	-0.020(5)	-0.011(5)	0.013(6)
C13	0.070(9)	0.055(9)	0.047(7)	-0.008(6)	0.001(6)	0.040(7)
C21	0.058(7)	0.019(5)	0.060(6)	0.000(5)	0.001(5)	0.003(5)
C22	0.064(8)	0.032(7)	0.111(9)	0.004(6)	-0.003(7)	0.008(6)
C23	0.048(7)	0.034(7)	0.091(8)	0.006(6)	-0.013(6)	-0.019(5)
C24	0.020(5)	0.074(7)	0.053(6)	-0.008(6)	0.006(4)	0.006(5)
C25	0.027(6)	0.116(11)	0.064(7)	-0.005(7)	0.013(5)	0.027(6)
C26	0.036(6)	0.127(12)	0.066(7)	0.022(8)	0.028(5)	-0.006(7)
C27	0.026(5)	0.055(7)	0.045(6)	0.001(5)	0.013(4)	-0.005(5)
C28	0.037(6)	0.030(6)	0.059(6)	0.001(5)	0.009(5)	0.009(5)

(b) within molecule B

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
BrB	0.0383(8)	0.0558(11)	0.1146(15)	-0.0082(10)	0.0204(9)	0.0008(7)
Mn	0.0299(8)	0.0329(9)	0.0405(8)	-0.0001(7)	0.0030(6)	-0.0050(7)
P1	0.0321(15)	0.0394(16)	0.0399(14)	-0.0014(12)	0.0046(11)	-0.0110(12)
O11	0.066(6)	0.076(6)	0.075(6)	0.007(5)	-0.001(5)	-0.024(5)
O12	0.062(5)	0.061(6)	0.071(5)	0.003(4)	-0.012(4)	-0.034(4)
O13B	0.101(11)	0.038(8)	0.096(12)	0.003(8)	0.040(9)	-0.005(7)
N1	0.027(4)	0.038(5)	0.032(4)	0.001(3)	0.010(3)	-0.007(4)
C1	0.043(6)	0.035(6)	0.050(6)	-0.001(5)	0.004(5)	-0.012(5)
C2	0.030(5)	0.031(6)	0.044(6)	0.000(5)	0.008(4)	-0.008(4)

Table 7aa. Anisotropic Displacement Parameters for **4**•0.5C_7H_8. (continued)

(b) within molecule B

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C3	0.030(5)	0.030(6)	0.025(4)	-0.005(4)	0.002(4)	0.004(4)
C3A	0.017(5)	0.020(5)	0.039(5)	-0.017(4)	0.007(4)	0.002(4)
C4	0.035(7)	0.051(8)	0.033(5)	-0.007(5)	0.003(4)	0.004(5)
C5	0.043(7)	0.043(7)	0.051(6)	-0.004(5)	0.015(5)	0.002(5)
C6	0.042(7)	0.059(8)	0.059(7)	-0.019(6)	0.001(5)	0.015(6)
C7	0.022(5)	0.044(7)	0.058(7)	-0.014(5)	0.007(5)	-0.006(5)
C7A	0.021(5)	0.041(6)	0.034(5)	-0.002(4)	0.002(4)	0.005(4)
C11	0.018(5)	0.061(8)	0.043(6)	0.003(6)	-0.005(5)	-0.008(5)
C12	0.044(7)	0.030(6)	0.049(6)	-0.001(5)	-0.004(5)	-0.003(5)
C13B	0.025(8)	0.061(11)	0.086(12)	0.009(9)	0.020(7)	0.017(7)
C21	0.038(7)	0.167(15)	0.037(6)	0.009(7)	0.014(5)	-0.025(8)
C22	0.044(8)	0.134(13)	0.109(11)	0.013(9)	0.034(7)	-0.025(8)
C23	0.027(7)	0.23(2)	0.092(10)	-0.095(12)	0.011(6)	-0.025(9)
C24	0.095(10)	0.037(7)	0.049(7)	0.008(5)	-0.011(6)	-0.020(7)
C25	0.166(15)	0.040(8)	0.078(9)	0.010(6)	0.010(9)	-0.042(9)
C26	0.098(13)	0.057(10)	0.142(13)	-0.041(9)	-0.065(11)	0.035(8)
C27	0.037(6)	0.030(6)	0.072(7)	0.009(5)	-0.002(5)	-0.004(5)
C28	0.036(6)	0.050(7)	0.053(6)	0.002(5)	0.016(5)	-0.007(5)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table 8aa. Derived Atomic Coordinates and Displacement Parameters for H-Atoms for **4**•0.5C_7H_8.

(a) hydrogen atoms of molecule A

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1AA	0.1032	0.1638	0.5122	0.044
H1BA	0.2184	0.2032	0.4677	0.044
H4A	-0.0816	0.2981	0.7574	0.050
H5A	0.1011	0.2837	0.9553	0.059
H6A	0.2991	0.2284	0.9558	0.054
H7A	0.3223	0.1860	0.7636	0.043
H21A	-0.1419	0.3531	0.5431	0.056
H22A	-0.2136	0.4118	0.3810	0.085
H22B	-0.3680	0.3834	0.4096	0.085
H22C	-0.2933	0.3742	0.2755	0.085
H23A	0.0561	0.3791	0.4223	0.073
H23B	0.0120	0.3389	0.3155	0.073
H23C	0.0875	0.3272	0.4677	0.073
H24A	-0.3532	0.3146	0.6141	0.058
H25A	-0.6348	0.3079	0.5474	0.082
H25B	-0.6081	0.2826	0.4121	0.082
H25C	-0.5568	0.3349	0.4355	0.082
H26A	-0.4814	0.2506	0.6902	0.089
H26B	-0.2965	0.2394	0.6799	0.089
H26C	-0.4385	0.2212	0.5669	0.089
H27A	0.1374	0.2020	0.2409	0.049
H27B	0.0760	0.2535	0.2186	0.049
H27C	0.0039	0.2148	0.1142	0.049
H28A	-0.0275	0.1449	0.3055	0.050
H28B	-0.1636	0.1560	0.1791	0.050
H28C	-0.2100	0.1545	0.3270	0.050

(b) hydrogen atoms of molecule B

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1AB	0.2081	0.1003	-0.0603	0.052
H1BB	0.0876	0.1388	-0.0179	0.052
H4B	-0.0917	0.0038	0.2279	0.048
H5B	0.0847	0.0181	0.4225	0.054
H6B	0.2882	0.0732	0.4271	0.065
H7B	0.3053	0.1171	0.2353	0.050
H21B	-0.3785	0.0008	0.0985	0.096
H22D	-0.6566	0.0081	0.0192	0.112
H22E	-0.5728	-0.0283	-0.0663	0.112
H22F	-0.6172	0.0215	-0.1260	0.112

Table 8aa. Derived Parameters for Hydrogen Atoms for **4**•0.5C_7H_8. (continued)

(b) hydrogen atoms of molecule B

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H23D	-0.5023	0.0680	0.1346	0.139
H23E	-0.4529	0.0886	-0.0002	0.139
H23F	-0.3153	0.0754	0.1232	0.139
H24B	-0.1931	-0.0515	0.0323	0.075
H25D	-0.2539	-0.1105	-0.1234	0.115
H25E	-0.2932	-0.0745	-0.2433	0.115
H25F	-0.4065	-0.0772	-0.1298	0.115
H26D	0.0192	-0.0818	-0.0626	0.130
H26E	0.0533	-0.0293	-0.0238	0.130
H26F	-0.0057	-0.0435	-0.1772	0.130
H27D	-0.0577	0.1572	-0.2180	0.057
H27E	-0.2388	0.1440	-0.2003	0.057
H27F	-0.1891	0.1454	-0.3470	0.057
H28D	0.1206	0.1027	-0.2861	0.054
H28E	-0.0093	0.0892	-0.4145	0.054
H28F	0.0674	0.0506	-0.3114	0.054

(c) hydrogen atoms of solvent toluene molecules

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H50A	0.8160	0.4143	0.7945	0.144[a]
H50B	0.7377	0.4640	0.7710	0.144[a]
H50C	0.7487	0.4315	0.6454	0.144[a]
H52	0.6468	0.3597	0.8742	0.087[a]
H53	0.3919	0.3294	0.8905	0.168[a]
H54	0.1576	0.3641	0.7764	0.109[a]
H55	0.1783	0.4292	0.6460	0.128[a]
H56	0.4332	0.4596	0.6297	0.132[a]
H60A	0.1503	0.3689	0.7669	0.122[b]
H60B	0.1439	0.3929	0.6236	0.122[b]
H60C	0.1322	0.4231	0.7540	0.122[b]
H62	0.4123	0.3435	0.8601	0.069[b]
H63	0.6950	0.3495	0.8927	0.128[b]
H64	0.8180	0.4105	0.7986	0.115[b]
H65	0.6583	0.4655	0.6718	0.112[b]
H66	0.3757	0.4596	0.6392	0.083[b]

[a]Derived with an occupancy factor of 0.6. [b]Derived with an occupancy factor of 0.4.

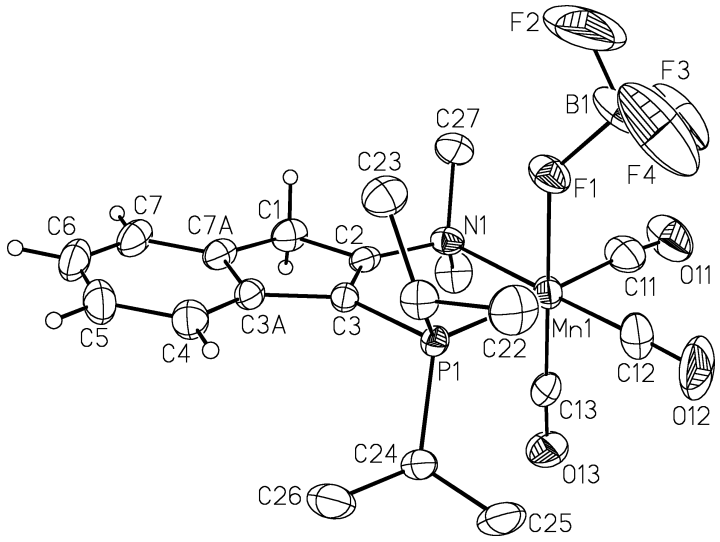

Figure 1b. Perspective view of one of the three crystallographically-independent molecules of [{κ^2–(2-Me$_2$N-1*H*-inden-3-yl)P^{i}Pr$_2$}Mn(CO)$_3$(FBF$_3$)] (molecule A) showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 50% probability level. Hydrogen atoms of the indenyl group are shown with arbitrarily small thermal parameters; all other hydrogens are not shown.

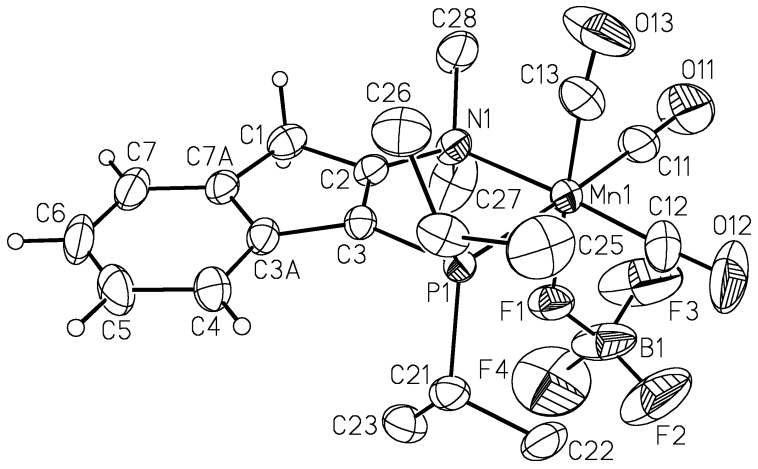

Figure 2b. View of the second crystallographically-independent molecule of [{κ^2–(2-Me$_2$N-1*H*-inden-3-yl)P^{i}Pr$_2$}Mn(CO)$_3$(FBF$_3$)] (molecule B).

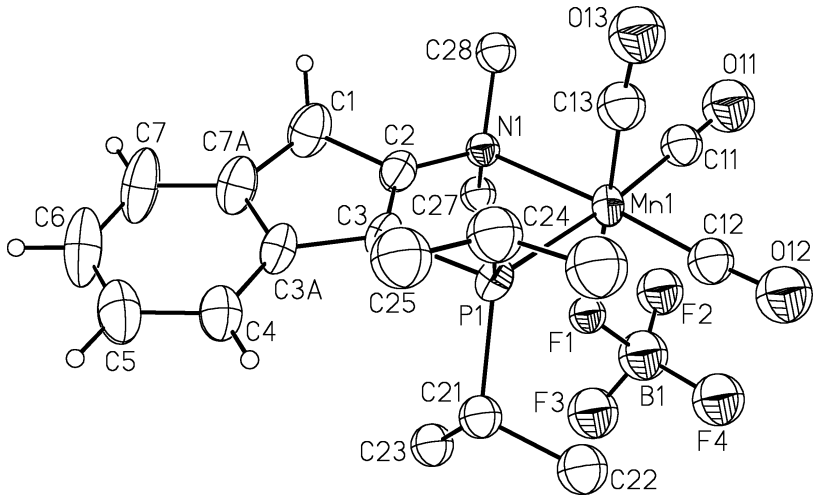

Figure 3b. View of the third crystallographically-independent molecule of [{κ^2–(2-Me$_2$N-1*H*-inden-3-yl)P^{i}Pr$_2$}Mn(CO)$_3$(FBF$_3$)] (molecule C).

Table 1b. Crystallographic Experimental Details for **5a**•$0.5C_7H_8$.

A. Crystal Data	
formula	$C_{23.5}H_{30}BF_4MnNO_3P$
formula weight	547.21
crystal dimensions (mm)	$0.62 \times 0.52 \times 0.16$
crystal system	monoclinic
space group	$P2_1/n$ (an alternate setting of $P2_1/c$ [No. 14])
unit cell parameters[a]	
a (Å)	8.1918 (6)
b (Å)	15.2453 (11)
c (Å)	62.102 (4)
β (deg)	93.4260 (14)
V (Å^3)	7741.8 (10)
Z	12
ρ_{calcd} (g cm^{-3})	1.408
μ (mm^{-1})	0.628
B. Data Collection and Refinement Conditions	
diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.3°) (10 s exposures)
data collection 2θ limit (deg)	52.78
total data collected	37759 ($-10 \le h \le 9$, $-19 \le k \le 15$, $-77 \le l \le 77$)
independent reflections	15801 (R_{int} = 0.0457)
number of observed reflections (*NO*)	11903 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	Patterson search/structure expansion (*DIRDIF–99*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	multi-scan (*SADABS*)
range of transmission factors	0.9063--0.6970
data/restraints/parameters	15801 [$F_o^2 \ge -3\sigma(F_o^2)$] / 3[e] / 911
goodness-of-fit (*S*)[f]	1.121 [$F_o^2 \ge -3\sigma(F_o^2)$]
final *R* indices[g]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0845
wR_2 [$F_o^2 \ge -3\sigma(F_o^2)$]	0.1918
largest difference peak and hole	1.045 and –0.996 e Å^{-3}

[a]Obtained from least-squares refinement of 6893 reflections with $4.76° < 2\theta < 48.69°$.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table 1b. Crystallographic Experimental Details for **5a**•$0.5C_7H_8$. (continued)

[c]Beurskens, P. T.; Beurskens, G.; de Gelder, R.; Garcia-Granda, S.; Israel, R.; Gould, R. O.; Smits, J. M. M. (1999). The *DIRDIF-99* program system. Crystallography Laboratory, University of Nijmegen, The Netherlands.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted *R*-factors wR_2 and all goodnesses of fit *S* are based on F_o^2; conventional *R*-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. *R*-factors based on F_o^2 are statistically about twice as large as those based on F_o, and *R*-factors based on ALL data will be even larger.

[e]Distances involving the methyl carbon of the inversion-disordered solvent toluene molecule were given fixed idealized values: d(C20S–C21S) = 1.54 Å; d(C20S···C22S) = d(C20S···C26S) = 2.54 Å. The aromatic ring of this molecule was refined as an idealized regular hexagon, with a fixed C–C bond length of 1.39 Å.

[f]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0411P)^2 + 26.9825P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[g]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2b. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for **5a**•0.5C_7H_8.

(a) [{κ²–(2-Me₂N-1H-inden-3-yl)P^{i}Pr₂}Mn(CO)₃(FBF₃)], molecule A

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Mn1	0.09235(8)	-0.15420(5)	0.246708(10)	0.02612(17)*
P1	0.04040(13)	-0.22450(7)	0.213508(17)	0.0213(2)*
F1	-0.0892(3)	-0.23117(19)	0.25876(4)	0.0389(7)*
F2	-0.2685(7)	-0.2789(5)	0.28218(8)	0.138(3)*
F3	-0.0379(6)	-0.2184(3)	0.29487(5)	0.0867(15)*
F4	-0.0416(9)	-0.3508(3)	0.27931(7)	0.129(2)*
O11	0.1528(5)	-0.0526(3)	0.28736(6)	0.0625(13)*
O12	0.3480(6)	-0.2799(3)	0.26167(7)	0.0706(14)*
O13	0.3540(4)	-0.0502(3)	0.22943(6)	0.0490(10)*
N1	-0.1008(4)	-0.0648(2)	0.23529(6)	0.0257(8)*
C1	-0.2935(6)	-0.0306(3)	0.20125(8)	0.0313(10)*
C2	-0.1633(5)	-0.0855(3)	0.21348(7)	0.0236(9)*
C3	-0.1221(5)	-0.1556(3)	0.20208(6)	0.0210(8)*
C3A	-0.2294(5)	-0.1603(3)	0.18212(7)	0.0249(9)*
C4	-0.2472(6)	-0.2224(3)	0.16586(7)	0.0342(11)*
C5	-0.3691(6)	-0.2112(4)	0.14956(8)	0.0397(12)*
C6	-0.4731(6)	-0.1397(4)	0.14956(8)	0.0436(13)*
C7	-0.4557(6)	-0.0772(3)	0.16552(8)	0.0374(12)*
C7A	-0.3337(5)	-0.0865(3)	0.18201(7)	0.0284(10)*
C11	0.1231(6)	-0.0924(4)	0.27239(8)	0.0413(12)*
C12	0.2462(7)	-0.2328(4)	0.25597(8)	0.0426(13)*
C13	0.2496(5)	-0.0906(3)	0.23591(7)	0.0314(10)*
C21	-0.0380(5)	-0.3382(3)	0.21186(7)	0.0284(9)*
C22	0.0659(7)	-0.4003(3)	0.22640(9)	0.0432(13)*
C23	-0.2182(6)	-0.3440(3)	0.21724(8)	0.0375(11)*
C24	0.2086(5)	-0.2161(3)	0.19479(7)	0.0283(10)*
C25	0.3669(6)	-0.2594(4)	0.20375(9)	0.0493(14)*
C26	0.1666(7)	-0.2473(4)	0.17179(8)	0.0463(14)*
C27	-0.2427(6)	-0.0701(4)	0.24949(8)	0.0404(12)*
C28	-0.0422(7)	0.0289(3)	0.23598(8)	0.0397(12)*
B1	-0.1064(11)	-0.2715(5)	0.27992(11)	0.059(2)*

(b) [{κ²–(2-Me₂N-1H-inden-3-yl)P^{i}Pr₂}Mn(CO)₃(FBF₃)], molecule B

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Mn1	-0.45473(9)	0.17119(5)	0.093389(12)	0.03523(19)*
P1	-0.33443(14)	0.22703(7)	0.125611(18)	0.0256(2)*
F1	-0.2582(4)	0.2247(2)	0.07884(4)	0.0469(8)*
F2	-0.2845(8)	0.3382(3)	0.05557(7)	0.120(2)*
F3	-0.3066(9)	0.2007(3)	0.04307(6)	0.134(3)*

Table 2b. Atomic Coordinates and Displacement Parameters for **5a**•0.5C_7H_8. (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
F4	-0.0696(8)	0.2548(5)	0.05573(9)	0.135(2)*
O11	-0.6095(8)	0.0929(4)	0.05337(8)	0.100(2)*
O12	-0.6558(7)	0.3282(4)	0.08451(10)	0.099(2)*
O13	-0.7428(6)	0.0992(4)	0.11262(9)	0.0897(18)*
N1	-0.2959(5)	0.0580(3)	0.10008(6)	0.0343(9)*
C1	-0.0873(6)	-0.0044(3)	0.13002(8)	0.0352(11)*
C2	-0.2010(6)	0.0659(3)	0.12063(7)	0.0282(10)*
C3	-0.2023(5)	0.1365(3)	0.13330(7)	0.0258(9)*
C3A	-0.0870(5)	0.1226(3)	0.15214(7)	0.0290(10)*
C4	-0.0426(6)	0.1756(4)	0.16951(7)	0.0388(12)*
C5	0.0745(7)	0.1443(4)	0.18485(8)	0.0498(15)*
C6	0.1438(7)	0.0628(4)	0.18267(9)	0.0503(15)*
C7	0.0978(6)	0.0096(4)	0.16535(9)	0.0428(13)*
C7A	-0.0187(5)	0.0395(3)	0.14992(8)	0.0319(10)*
C11	-0.5406(8)	0.1223(4)	0.06814(10)	0.0598(18)*
C12	-0.5752(8)	0.2684(4)	0.08818(10)	0.0571(16)*
C13	-0.6257(8)	0.1265(4)	0.10584(10)	0.0558(16)*
C21	-0.2024(6)	0.3256(3)	0.12504(7)	0.0343(11)*
C22	-0.2854(7)	0.3996(3)	0.11177(9)	0.0474(14)*
C23	-0.0326(7)	0.3071(4)	0.11724(9)	0.0485(14)*
C24	-0.4534(6)	0.2455(3)	0.14969(9)	0.0400(12)*
C25	-0.6003(8)	0.3059(5)	0.14476(12)	0.070(2)*
C26	-0.5077(7)	0.1602(4)	0.15965(9)	0.0522(15)*
C27	-0.1763(9)	0.0467(5)	0.08290(9)	0.071(2)*
C28	-0.3945(9)	-0.0240(4)	0.10076(11)	0.070(2)*
B1	-0.2326(13)	0.2566(6)	0.05710(11)	0.071(3)*

(c) [{κ^2–(2-Me_2N-1H-inden-3-yl)P^iPr_2}Mn(CO)$_3$(FBF_3)], molecule C

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Mn1[a]	0.2318(8)	-0.3530(5)	0.07757(8)	0.0340(9)*
Mn1'[a]	0.2551(9)	-0.3428(5)	0.07211(9)	0.0408(11)*
P1[a]	0.179(2)	-0.2832(10)	0.0442(3)	0.031(2)*
P1'[a]	0.164(2)	-0.2659(10)	0.0412(3)	0.0305(19)*
F1[a]	0.0458(8)	-0.2766(4)	0.08927(10)	0.0307(16)
F2[a]	-0.0003(10)	-0.3132(5)	0.12319(11)	0.0548(18)
F3[a]	-0.1268(13)	-0.2010(7)	0.10805(16)	0.065(3)
F4[a]	0.1435(13)	-0.1807(7)	0.11644(16)	0.063(3)
F1'[a]	0.0968(9)	-0.2678(5)	0.08816(11)	0.0400(19)
F2'[a]	0.0946(12)	-0.3113(6)	0.12363(15)	0.084(3)
F3'[a]	-0.0706(18)	-0.1973(11)	0.1110(2)	0.112(5)

Table 2b. Atomic Coordinates and Displacement Parameters for **5a**•0.5C_7H_8. (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
F4'[a]	0.1919(19)	-0.1911(11)	0.1156(3)	0.125(6)
O11[a]	0.2958(12)	-0.4563(6)	0.11748(16)	0.064(3)
O12[a]	0.4900(12)	-0.2305(6)	0.09302(16)	0.061(2)
O13[a]	0.4895(11)	-0.4602(6)	0.06061(16)	0.060(2)
O11'[a]	0.3724(15)	-0.4463(8)	0.11084(19)	0.082(3)
O12'[a]	0.5257(14)	-0.2180(8)	0.08247(19)	0.081(3)
O13'[a]	0.4982(11)	-0.4427(6)	0.05006(16)	0.059(2)
N1[a]	0.0316(16)	-0.4401(8)	0.0652(2)	0.025(3)
N1'[a]	0.0595(18)	-0.4315(10)	0.0641(2)	0.042(5)
C1	-0.1398(7)	-0.4785(4)	0.03049(9)	0.0496(14)*
C2	-0.0187(6)	-0.4197(3)	0.04292(8)	0.0349(11)*
C3	0.0160(6)	-0.3479(3)	0.03170(7)	0.0330(10)*
C3A	-0.0879(6)	-0.3471(4)	0.01133(7)	0.0373(11)*
C4	-0.1056(7)	-0.2864(4)	-0.00531(8)	0.0471(14)*
C5	-0.2213(8)	-0.3021(5)	-0.02215(9)	0.0595(17)*
C6	-0.3134(8)	-0.3769(6)	-0.02237(10)	0.074(2)*
C7	-0.2956(8)	-0.4383(5)	-0.00634(10)	0.068(2)*
C7A	-0.1810(7)	-0.4240(4)	0.01080(9)	0.0505(15)*
C11[a]	0.2650(15)	-0.4154(8)	0.10221(19)	0.039(3)
C12[a]	0.3825(15)	-0.2772(8)	0.0870(2)	0.042(3)
C13[a]	0.3820(15)	-0.4176(9)	0.0668(2)	0.046(3)
C21[a]	0.1006(16)	-0.1676(8)	0.04276(19)	0.035(3)
C22[a]	0.2011(18)	-0.1078(9)	0.0588(2)	0.048(4)
C23[a]	-0.0807(17)	-0.1635(9)	0.0475(2)	0.038(3)
C24[a]	0.3476(15)	-0.2924(9)	0.0259(2)	0.054(3)
C25[a]	0.3089(16)	-0.2733(10)	0.0036(2)	0.060(3)
C26[a]	0.5003(16)	-0.2416(9)	0.0340(2)	0.062(3)
C27[a]	-0.1120(18)	-0.4240(9)	0.0787(2)	0.031(3)
C28[a]	0.0807(16)	-0.5320(9)	0.0687(2)	0.036(3)
C11'[a]	0.3195(18)	-0.4035(9)	0.0959(2)	0.057(3)
C12'[a]	0.4184(18)	-0.2676(10)	0.0791(2)	0.058(4)
C13'[a]	0.4003(15)	-0.4032(8)	0.0586(2)	0.041(3)
C21'[a]	0.0508(16)	-0.1609(8)	0.04427(19)	0.032(3)
C22'[a]	0.1477(18)	-0.0974(10)	0.0587(2)	0.049(4)
C23'[a]	-0.1209(17)	-0.1734(10)	0.0506(2)	0.045(4)
C24'[a]	0.2985(12)	-0.2467(7)	0.01864(17)	0.036(2)
C25'[a]	0.3308(13)	-0.3317(8)	0.00584(17)	0.043(2)
C26'[a]	0.4521(16)	-0.2000(9)	0.0263(2)	0.062(3)
C27'[a]	-0.075(2)	-0.4306(14)	0.0793(4)	0.071(7)
C28'[a]	0.115(2)	-0.5280(12)	0.0640(3)	0.066(5)

Table 2b. Atomic Coordinates and Displacement Parameters for **5a**•0.5C_7H_8. (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
B1[a]	0.006(3)	-0.2438(13)	0.1118(3)	0.060(5)
B1'[a]	0.066(2)	-0.2413(10)	0.1102(2)	0.043(4)

(d) solvent toluene atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C10S	-0.4408(11)	-0.4565(6)	0.16472(14)	0.096(3)*
C11S	-0.2721(9)	-0.4914(4)	0.16774(10)	0.0598(17)*
C12S	-0.1518(12)	-0.4598(5)	0.15556(12)	0.076(2)*
C13S	0.0030(13)	-0.4911(7)	0.15851(16)	0.098(3)*
C14S	0.0441(12)	-0.5535(8)	0.1736(2)	0.112(4)*
C15S	-0.0803(14)	-0.5870(6)	0.18592(14)	0.097(3)*
C16S	-0.2371(11)	-0.5563(5)	0.18274(11)	0.071(2)*
C20S[a,b]	0.3038(8)	-0.0149(9)	-0.0123(2)	0.0743(16)
C21S[a,b]	0.1309(8)	-0.0039(7)	-0.00420(16)	0.0743(16)
C22S[a,b]	-0.0005(9)	-0.0482(7)	-0.01439(15)	0.0743(16)
C23S[a,b]	-0.1572(8)	-0.0362(7)	-0.00749(17)	0.0743(16)
C24S[a,b]	-0.1827(9)	0.0201(7)	0.00961(17)	0.0743(16)
C25S[a,b]	-0.0513(11)	0.0643(7)	0.01980(15)	0.0743(16)
C26S[a,b]	0.1055(10)	0.0523(7)	0.01290(15)	0.0743(16)

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$. [a]Refined with an occupancy factor of 0.5. [b]Carbon atoms of this inversion-disordered solvent toluene molecule were refined with a common isotropic displacement parameter.

Table 3b. Selected Interatomic Distances (Å) for **5a**•0.5C_7H_8.

(a) [{κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}Mn(CO)$_3$(FBF_3)], molecule A

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Mn1	P1	2.3401(13)	N1	C27	1.503(6)
Mn1	F1	2.070(3)	N1	C28	1.507(6)
Mn1	N1	2.175(4)	C1	C2	1.523(6)
Mn1	C11	1.857(5)	C1	C7A	1.489(7)
Mn1	C12	1.808(5)	C2	C3	1.336(6)
Mn1	C13	1.776(5)	C3	C3A	1.477(5)
P1	C3	1.808(4)	C3A	C4	1.385(6)
P1	C21	1.849(5)	C3A	C7A	1.412(6)
P1	C24	1.859(4)	C4	C5	1.389(7)
F1	B1	1.465(7)	C5	C6	1.383(8)
F2	B1	1.348(10)	C6	C7	1.377(8)
F3	B1	1.330(8)	C7	C7A	1.395(6)
F4	B1	1.323(9)	C21	C22	1.532(6)
O11	C11	1.125(6)	C21	C23	1.536(6)
O12	C12	1.141(6)	C24	C25	1.529(6)
O13	C13	1.146(6)	C24	C26	1.525(6)
N1	C2	1.454(5)			

(b) [{κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}Mn(CO)$_3$(FBF_3)], molecule B

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Mn1	P1	2.3376(13)	N1	C27	1.501(7)
Mn1	F1	2.061(3)	N1	C28	1.491(7)
Mn1	N1	2.186(4)	C1	C2	1.513(6)
Mn1	C11	1.838(6)	C1	C7A	1.486(7)
Mn1	C12	1.799(6)	C2	C3	1.334(6)
Mn1	C13	1.776(7)	C3	C3A	1.474(6)
P1	C3	1.801(5)	C3A	C4	1.379(7)
P1	C21	1.853(5)	C3A	C7A	1.395(7)
P1	C24	1.855(5)	C4	C5	1.395(7)
F1	B1	1.462(7)	C5	C6	1.375(9)
F2	B1	1.318(10)	C6	C7	1.381(8)
F3	B1	1.338(9)	C7	C7A	1.388(7)
F4	B1	1.343(11)	C21	C22	1.532(7)
O11	C11	1.139(7)	C21	C23	1.526(7)
O12	C12	1.141(7)	C24	C25	1.531(8)
O13	C13	1.148(7)	C24	C26	1.518(8)
N1	C2	1.459(6)			

Table 3b. Selected Interatomic Distances for **5a**•0.5C_7H_8. (continued)

(c) [{κ²–(2-Me₂N-1H-inden-3-yl)P^{i}Pr₂}Mn(CO)₃(FBF₃)], molecule C

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Mn1	P1	2.344(13)	O13	C13	1.178(15)
Mn1	F1	2.082(10)	O11’	C11’	1.196(17)
Mn1	N1	2.212(14)	O12’	C12’	1.169(17)
Mn1	C11	1.809(13)	O13’	C13’	1.157(14)
Mn1	C12	1.765(14)	N1	C2	1.453(13)
Mn1	C13	1.740(15)	N1	C27	1.506(19)
Mn1’	P1’	2.334(13)	N1	C28	1.470(18)
Mn1’	F1’	2.034(10)	N1’	C2	1.442(16)
Mn1’	N1’	2.133(16)	N1’	C27’	1.49(2)
Mn1’	C11’	1.793(15)	N1’	C28’	1.54(2)
Mn1’	C12’	1.796(17)	C1	C2	1.514(7)
Mn1’	C13’	1.756(14)	C1	C7A	1.500(8)
P1	C3	1.80(2)	C2	C3	1.338(7)
P1	C21	1.876(18)	C3	C3A	1.482(6)
P1	C24	1.85(2)	C3A	C4	1.388(7)
P1’	C3	1.81(2)	C3A	C7A	1.397(7)
P1’	C21’	1.86(2)	C4	C5	1.390(8)
P1’	C24’	1.86(2)	C5	C6	1.367(10)
F1	B1	1.54(2)	C6	C7	1.369(10)
F2	B1	1.27(2)	C7	C7A	1.394(8)
F3	B1	1.28(3)	C21	C22	1.549(18)
F4	B1	1.49(2)	C21	C23	1.533(17)
F1’	B1’	1.463(17)	C24	C25	1.435(17)
F2’	B1’	1.368(17)	C24	C26	1.529(17)
F3’	B1’	1.31(2)	C21’	C22’	1.512(18)
F4’	B1’	1.31(2)	C21’	C23’	1.496(18)
O11	C11	1.150(14)	C24’	C25’	1.551(15)
O12	C12	1.175(14)	C24’	C26’	1.497(16)

(d) within the solvent toluene molecules

Atom1	Atom2	Distance	Atom1	Atom2	Distance
C10S	C11S	1.482(10)	C20S	C21S	1.54†
C11S	C12S	1.365(10)	C21S	C22S	1.39†
C11S	C16S	1.378(10)	C21S	C26S	1.39†
C12S	C13S	1.358(12)	C22S	C23S	1.39†
C13S	C14S	1.363(14)	C23S	C24S	1.39†
C14S	C15S	1.407(15)	C24S	C25S	1.39†
C15S	C16S	1.370(11)	C25S	C26S	1.39†

†Distance fixed during refinement.

Table 4b. Selected Interatomic Angles (deg) for **5a**•0.5C_7H_8.

(a) [{κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}Mn(CO)$_3$(FBF_3)], molecule A

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
P1	Mn1	F1	87.83(8)	N1	C2	C3	125.6(4)
P1	Mn1	N1	84.80(10)	C1	C2	C3	111.5(4)
P1	Mn1	C11	175.98(19)	P1	C3	C2	117.4(3)
P1	Mn1	C12	93.63(17)	P1	C3	C3A	133.5(3)
P1	Mn1	C13	90.86(15)	C2	C3	C3A	109.1(4)
F1	Mn1	N1	87.06(13)	C3	C3A	C4	132.6(4)
F1	Mn1	C11	92.32(17)	C3	C3A	C7A	107.2(4)
F1	Mn1	C12	90.7(2)	C4	C3A	C7A	120.2(4)
F1	Mn1	C13	178.42(19)	C3A	C4	C5	119.2(5)
N1	Mn1	C11	91.2(2)	C4	C5	C6	120.8(5)
N1	Mn1	C12	177.3(2)	C5	C6	C7	120.6(4)
N1	Mn1	C13	93.72(18)	C6	C7	C7A	119.8(5)
C11	Mn1	C12	90.4(2)	C1	C7A	C3A	110.3(4)
C11	Mn1	C13	89.0(2)	C1	C7A	C7	130.2(4)
C12	Mn1	C13	88.5(2)	C3A	C7A	C7	119.5(4)
Mn1	P1	C3	99.82(14)	Mn1	C11	O11	174.6(5)
Mn1	P1	C21	121.49(15)	Mn1	C12	O12	177.2(6)
Mn1	P1	C24	114.62(15)	Mn1	C13	O13	178.1(4)
C3	P1	C21	106.13(19)	P1	C21	C22	111.6(3)
C3	P1	C24	105.70(19)	P1	C21	C23	112.2(3)
C21	P1	C24	107.3(2)	C22	C21	C23	110.1(4)
Mn1	F1	B1	132.2(4)	P1	C24	C25	112.8(3)
Mn1	N1	C2	112.1(3)	P1	C24	C26	115.5(3)
Mn1	N1	C27	110.4(3)	C25	C24	C26	110.2(4)
Mn1	N1	C28	111.1(3)	F1	B1	F2	106.1(7)
C2	N1	C27	107.1(3)	F1	B1	F3	108.2(5)
C2	N1	C28	109.0(3)	F1	B1	F4	107.3(5)
C27	N1	C28	106.9(4)	F2	B1	F3	110.8(6)
C2	C1	C7A	101.5(4)	F2	B1	F4	109.0(6)
N1	C2	C1	122.8(4)	F3	B1	F4	115.0(8)

(b) [{κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}Mn(CO)$_3$(FBF_3)], molecule B

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
P1	Mn1	F1	86.03(9)	N1	Mn1	C11	92.0(2)
P1	Mn1	N1	84.77(10)	N1	Mn1	C12	176.6(2)
P1	Mn1	C11	176.8(2)	N1	Mn1	C13	95.2(2)
P1	Mn1	C12	93.0(2)	C11	Mn1	C12	90.2(3)
P1	Mn1	C13	94.02(19)	C11	Mn1	C13	86.8(3)
F1	Mn1	N1	85.63(15)	C12	Mn1	C13	87.5(3)
F1	Mn1	C11	93.2(2)	Mn1	P1	C3	99.43(14)
F1	Mn1	C12	91.7(2)	Mn1	P1	C21	119.71(15)
F1	Mn1	C13	179.2(2)	Mn1	P1	C24	122.03(17)

Table 4b. Selected Interatomic Angles for **5a**•0.5C_7H_8. (continued)

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C3	P1	C21	106.5(2)	C4	C5	C6	120.8(5)
C3	P1	C24	103.8(2)	C5	C6	C7	120.8(5)
C21	P1	C24	103.2(2)	C6	C7	C7A	119.2(5)
Mn1	F1	B1	134.1(4)	C1	C7A	C3A	110.9(4)
Mn1	N1	C2	112.4(3)	C1	C7A	C7	129.5(5)
Mn1	N1	C27	111.2(3)	C3A	C7A	C7	119.6(5)
Mn1	N1	C28	110.5(4)	Mn1	C11	O11	172.8(7)
C2	N1	C27	107.1(4)	Mn1	C12	O12	177.6(6)
C2	N1	C28	107.8(4)	Mn1	C13	O13	175.2(6)
C27	N1	C28	107.5(5)	P1	C21	C22	111.5(3)
C2	C1	C7A	101.3(4)	P1	C21	C23	113.6(4)
N1	C2	C1	124.2(4)	C22	C21	C23	110.4(4)
N1	C2	C3	124.0(4)	P1	C24	C25	112.0(4)
C1	C2	C3	111.8(4)	P1	C24	C26	112.3(4)
P1	C3	C2	119.2(3)	C25	C24	C26	110.5(5)
P1	C3	C3A	131.8(3)	F1	B1	F2	108.5(6)
C2	C3	C3A	109.0(4)	F1	B1	F3	107.8(5)
C3	C3A	C4	131.6(4)	F1	B1	F4	104.5(7)
C3	C3A	C7A	107.1(4)	F2	B1	F3	115.0(9)
C4	C3A	C7A	121.4(4)	F2	B1	F4	109.4(7)
C3A	C4	C5	118.2(5)	F3	B1	F4	111.1(8)

(c) [{ κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}Mn(CO)$_3$(FBF_3)], molecule C

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
P1	Mn1	F1	87.4(5)	P1’	Mn1’	C13’	93.7(6)
P1	Mn1	N1	82.6(6)	F1’	Mn1’	N1’	88.8(5)
P1	Mn1	C11	175.0(7)	F1’	Mn1’	C11’	93.0(6)
P1	Mn1	C12	94.9(7)	F1’	Mn1’	C12’	90.5(6)
P1	Mn1	C13	90.9(6)	F1’	Mn1’	C13’	176.8(7)
F1	Mn1	N1	85.1(4)	N1’	Mn1’	C11’	92.5(7)
F1	Mn1	C11	94.3(5)	N1’	Mn1’	C12’	179.3(8)
F1	Mn1	C12	91.7(6)	N1’	Mn1’	C13’	94.5(7)
F1	Mn1	C13	177.6(6)	C11’	Mn1’	C12’	87.3(7)
N1	Mn1	C11	92.8(5)	C11’	Mn1’	C13’	87.0(7)
N1	Mn1	C12	176.1(7)	C12’	Mn1’	C13’	86.2(7)
N1	Mn1	C13	93.0(6)	Mn1	P1	C3	103.1(7)
C11	Mn1	C12	89.8(6)	Mn1	P1	C21	120.9(10)
C11	Mn1	C13	87.3(7)	Mn1	P1	C24	113.8(8)
C12	Mn1	C13	90.1(6)	C3	P1	C21	104.5(8)
P1’	Mn1’	F1’	86.4(6)	C3	P1	C24	104.8(10)
P1’	Mn1’	N1’	85.9(7)	C21	P1	C24	107.9(10)
P1’	Mn1’	C11’	178.3(8)	Mn1’	P1’	C3	95.5(7)
P1’	Mn1’	C12’	94.3(7)	Mn1’	P1’	C21’	119.0(10)

Table 4b. Selected Interatomic Angles for **5a**•0.5C_7H_8. (continued)

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
Mn1’	P1’	C24’	121.5(9)	C6	C7	C7A	119.1(6)
C3	P1’	C21’	107.4(9)	C1	C7A	C3A	110.5(5)
C3	P1’	C24’	106.1(10)	C1	C7A	C7	130.1(6)
C21’	P1’	C24’	105.2(8)	C3A	C7A	C7	119.4(6)
Mn1	F1	B1	134.3(9)	Mn1	C11	O11	175.7(12)
Mn1’	F1’	B1’	139.9(8)	Mn1	C12	O12	175.8(12)
Mn1	N1	C2	111.4(7)	Mn1	C13	O13	176.1(12)
Mn1	N1	C27	107.2(9)	P1	C21	C22	110.8(10)
Mn1	N1	C28	109.3(9)	P1	C21	C23	111.2(10)
C2	N1	C27	108.0(9)	C22	C21	C23	109.6(11)
C2	N1	C28	114.0(10)	P1	C24	C25	116.8(11)
C27	N1	C28	106.7(11)	P1	C24	C26	112.8(11)
Mn1’	N1’	C2	114.8(9)	C25	C24	C26	110.1(11)
Mn1’	N1’	C27’	114.8(12)	Mn1’	C11’	O11’	174.9(14)
Mn1’	N1’	C28’	112.9(11)	Mn1’	C12’	O12’	176.3(15)
C2	N1’	C27’	105.8(12)	Mn1’	C13’	O13’	178.7(12)
C2	N1’	C28’	103.2(12)	P1’	C21’	C22’	111.3(11)
C27’	N1’	C28’	104.1(14)	P1’	C21’	C23’	113.4(11)
C2	C1	C7A	101.3(4)	C22’	C21’	C23’	113.2(11)
N1	C2	C1	119.9(6)	P1’	C24’	C25’	112.5(9)
N1	C2	C3	127.9(6)	P1’	C24’	C26’	111.2(10)
N1’	C2	C1	129.3(7)	C25’	C24’	C26’	113.2(9)
N1’	C2	C3	118.8(7)	F1	B1	F2	104.5(14)
C1	C2	C3	111.9(4)	F1	B1	F3	102.9(13)
P1	C3	C2	113.5(5)	F1	B1	F4	100.6(14)
P1	C3	C3A	137.6(6)	F2	B1	F3	117.6(18)
P1’	C3	C2	123.6(6)	F2	B1	F4	118.9(16)
P1’	C3	C3A	127.6(6)	F3	B1	F4	109.3(16)
C2	C3	C3A	108.8(4)	F1’	B1’	F2’	108.8(11)
C3	C3A	C4	132.0(5)	F1’	B1’	F3’	111.9(12)
C3	C3A	C7A	107.4(5)	F1’	B1’	F4’	102.9(14)
C4	C3A	C7A	120.6(5)	F2’	B1’	F3’	119.6(16)
C3A	C4	C5	118.8(6)	F2’	B1’	F4’	101.2(14)
C4	C5	C6	120.1(6)	F3’	B1’	F4’	110.7(15)
C5	C6	C7	121.9(6)				

(d) within the solvent toluene molecules

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C10S	C11S	C12S	120.1(8)	C13S	C14S	C15S	118.1(9)
C10S	C11S	C16S	119.9(8)	C14S	C15S	C16S	120.0(10)
C12S	C11S	C16S	120.0(8)	C11S	C16S	C15S	119.9(8)
C11S	C12S	C13S	120.1(9)	C20S	C21S	C22S	120.0†
C12S	C13S	C14S	121.9(10)	C20S	C21S	C26S	120.0†

Table 4b. Selected Interatomic Angles for **5a**•0.5C_7H_8. (continued)

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C22S	C21S	C26S	120.0†	C23S	C24S	C25S	120.0†
C21S	C22S	C23S	120.0†	C24S	C25S	C26S	120.0†
C22S	C23S	C24S	120.0†	C21S	C26S	C25S	120.0†

†Angle fixed during refinement.

Table 5b. Torsional Angles (deg) for **5a**•0.5C_7H_8.

(a) [{κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}Mn(CO)$_3$(FBF_3)], molecule A

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
F1	Mn1	P1	C3	87.07(16)	C13	Mn1	C11	O11	-13(6)
F1	Mn1	P1	C21	-28.83(19)	P1	Mn1	C12	O12	105(10)
F1	Mn1	P1	C24	-160.51(18)	F1	Mn1	C12	O12	-167(100)
N1	Mn1	P1	C3	-0.17(16)	N1	Mn1	C12	O12	160(8)
N1	Mn1	P1	C21	-116.06(19)	C11	Mn1	C12	O12	-75(10)
N1	Mn1	P1	C24	112.25(19)	C13	Mn1	C12	O12	14(10)
C11	Mn1	P1	C3	-5(2)	P1	Mn1	C13	O13	-132(16)
C11	Mn1	P1	C21	-121(2)	F1	Mn1	C13	O13	-98(18)
C11	Mn1	P1	C24	107(2)	N1	Mn1	C13	O13	143(16)
C12	Mn1	P1	C3	177.6(2)	C11	Mn1	C13	O13	52(16)
C12	Mn1	P1	C21	61.7(2)	C12	Mn1	C13	O13	-38(16)
C12	Mn1	P1	C24	-70.0(2)	Mn1	P1	C3	C2	3.4(3)
C13	Mn1	P1	C3	-93.8(2)	Mn1	P1	C3	C3A	-174.6(4)
C13	Mn1	P1	C21	150.3(2)	C21	P1	C3	C2	130.4(3)
C13	Mn1	P1	C24	18.6(2)	C21	P1	C3	C3A	-47.6(4)
P1	Mn1	F1	B1	144.4(5)	C24	P1	C3	C2	-115.8(3)
N1	Mn1	F1	B1	-130.7(5)	C24	P1	C3	C3A	66.2(4)
C11	Mn1	F1	B1	-39.7(5)	Mn1	P1	C21	C22	-51.5(4)
C12	Mn1	F1	B1	50.8(5)	Mn1	P1	C21	C23	72.6(3)
C13	Mn1	F1	B1	110(7)	C3	P1	C21	C22	-164.1(3)
P1	Mn1	N1	C2	-2.7(3)	C3	P1	C21	C23	-40.0(4)
P1	Mn1	N1	C27	116.6(3)	C24	P1	C21	C22	83.2(4)
P1	Mn1	N1	C28	-125.0(3)	C24	P1	C21	C23	-152.7(3)
F1	Mn1	N1	C2	-90.8(3)	Mn1	P1	C24	C25	62.3(4)
F1	Mn1	N1	C27	28.5(3)	Mn1	P1	C24	C26	-169.8(3)
F1	Mn1	N1	C28	146.9(3)	C3	P1	C24	C25	171.2(4)
C11	Mn1	N1	C2	177.0(3)	C3	P1	C24	C26	-60.9(4)
C11	Mn1	N1	C27	-63.8(3)	C21	P1	C24	C25	-75.8(4)
C11	Mn1	N1	C28	54.6(3)	C21	P1	C24	C26	52.0(4)
C12	Mn1	N1	C2	-58(4)	Mn1	F1	B1	F2	152.8(4)
C12	Mn1	N1	C27	62(4)	Mn1	F1	B1	F3	33.9(9)
C12	Mn1	N1	C28	-180(100)	Mn1	F1	B1	F4	-90.8(6)
C13	Mn1	N1	C2	87.8(3)	Mn1	N1	C2	C1	-177.1(3)
C13	Mn1	N1	C27	-152.9(3)	Mn1	N1	C2	C3	6.4(5)
C13	Mn1	N1	C28	-34.5(3)	C27	N1	C2	C1	61.7(5)
P1	Mn1	C11	O11	-102(6)	C27	N1	C2	C3	-114.8(5)
F1	Mn1	C11	O11	166(6)	C28	N1	C2	C1	-53.6(5)
N1	Mn1	C11	O11	-107(6)	C28	N1	C2	C3	129.9(5)
C12	Mn1	C11	O11	75(6)	C7A	C1	C2	N1	-170.7(4)

Table 5b. Torsional Angles for **5a**•0.5C_7H_8. (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C7A	C1	C2	C3	6.2(5)	C3	C3A	C4	C5	175.4(4)
C2	C1	C7A	C3A	-4.8(5)	C7A	C3A	C4	C5	-0.2(7)
C2	C1	C7A	C7	173.0(5)	C3	C3A	C7A	C1	2.1(5)
N1	C2	C3	P1	-6.9(6)	C3	C3A	C7A	C7	-176.0(4)
N1	C2	C3	C3A	171.6(4)	C4	C3A	C7A	C1	178.7(4)
C1	C2	C3	P1	176.3(3)	C4	C3A	C7A	C7	0.6(6)
C1	C2	C3	C3A	-5.3(5)	C3A	C4	C5	C6	-0.8(7)
P1	C3	C3A	C4	4.1(8)	C4	C5	C6	C7	1.4(8)
P1	C3	C3A	C7A	-179.9(3)	C5	C6	C7	C7A	-0.9(7)
C2	C3	C3A	C4	-174.0(5)	C6	C7	C7A	C1	-177.7(5)
C2	C3	C3A	C7A	2.0(5)	C6	C7	C7A	C3A	-0.1(7)

(b) [{κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}Mn(CO)$_3$(FBF_3)], molecule B

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
F1	Mn1	P1	C3	-87.55(17)	C11	Mn1	N1	C2	-177.5(4)
F1	Mn1	P1	C21	27.7(2)	C11	Mn1	N1	C27	62.3(4)
F1	Mn1	P1	C24	159.5(2)	C11	Mn1	N1	C28	-57.1(4)
N1	Mn1	P1	C3	-1.58(18)	C12	Mn1	N1	C2	52(4)
N1	Mn1	P1	C21	113.7(2)	C12	Mn1	N1	C27	-68(4)
N1	Mn1	P1	C24	-114.5(2)	C12	Mn1	N1	C28	172(100)
C11	Mn1	P1	C3	-11(4)	C13	Mn1	N1	C2	-90.6(3)
C11	Mn1	P1	C21	104(4)	C13	Mn1	N1	C27	149.3(4)
C11	Mn1	P1	C24	-124(4)	C13	Mn1	N1	C28	29.9(4)
C12	Mn1	P1	C3	-179.1(3)	P1	Mn1	C11	O11	133(4)
C12	Mn1	P1	C21	-63.8(3)	F1	Mn1	C11	O11	-151(5)
C12	Mn1	P1	C24	68.0(3)	N1	Mn1	C11	O11	123(5)
C13	Mn1	P1	C3	93.3(3)	C12	Mn1	C11	O11	-60(5)
C13	Mn1	P1	C21	-151.5(3)	C13	Mn1	C11	O11	28(5)
C13	Mn1	P1	C24	-19.7(3)	P1	Mn1	C12	O12	-149(18)
P1	Mn1	F1	B1	-153.4(6)	F1	Mn1	C12	O12	124(18)
N1	Mn1	F1	B1	121.5(6)	N1	Mn1	C12	O12	162(100)
C11	Mn1	F1	B1	29.7(6)	C11	Mn1	C12	O12	31(18)
C12	Mn1	F1	B1	-60.5(6)	C13	Mn1	C12	O12	-56(18)
C13	Mn1	F1	B1	-60(15)	P1	Mn1	C13	O13	143(8)
P1	Mn1	N1	C2	3.0(3)	F1	Mn1	C13	O13	50(20)
P1	Mn1	N1	C27	-117.1(4)	N1	Mn1	C13	O13	-132(8)
P1	Mn1	N1	C28	123.5(4)	C11	Mn1	C13	O13	-40(8)
F1	Mn1	N1	C2	89.4(3)	C12	Mn1	C13	O13	50(8)
F1	Mn1	N1	C27	-30.7(4)	Mn1	P1	C3	C2	0.1(4)
F1	Mn1	N1	C28	-150.1(4)	Mn1	P1	C3	C3A	-179.6(4)

Table 5b. Torsional Angles for **5a**•0.5C_7H_8. (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C21	P1	C3	C2	-124.9(4)	C28	N1	C2	C3	-126.2(5)
C21	P1	C3	C3A	55.4(5)	C7A	C1	C2	N1	177.2(4)
C24	P1	C3	C2	126.6(4)	C7A	C1	C2	C3	-2.0(5)
C24	P1	C3	C3A	-53.1(5)	C2	C1	C7A	C3A	1.7(5)
Mn1	P1	C21	C22	49.5(4)	C2	C1	C7A	C7	-177.9(5)
Mn1	P1	C21	C23	-76.0(4)	N1	C2	C3	P1	2.7(6)
C3	P1	C21	C22	161.0(4)	N1	C2	C3	C3A	-177.6(4)
C3	P1	C21	C23	35.4(4)	C1	C2	C3	P1	-178.1(3)
C24	P1	C21	C22	-90.1(4)	C1	C2	C3	C3A	1.6(5)
C24	P1	C21	C23	144.4(4)	P1	C3	C3A	C4	-1.4(8)
Mn1	P1	C24	C25	-56.2(5)	P1	C3	C3A	C7A	179.2(4)
Mn1	P1	C24	C26	68.8(4)	C2	C3	C3A	C4	179.0(5)
C3	P1	C24	C25	-166.9(4)	C2	C3	C3A	C7A	-0.5(5)
C3	P1	C24	C26	-41.8(4)	C3	C3A	C4	C5	-178.7(5)
C21	P1	C24	C25	82.1(4)	C7A	C3A	C4	C5	0.6(7)
C21	P1	C24	C26	-152.8(4)	C3	C3A	C7A	C1	-0.9(5)
Mn1	F1	B1	F2	83.9(7)	C3	C3A	C7A	C7	178.8(4)
Mn1	F1	B1	F3	-41.3(11)	C4	C3A	C7A	C1	179.6(4)
Mn1	F1	B1	F4	-159.5(4)	C4	C3A	C7A	C7	-0.7(7)
Mn1	N1	C2	C1	176.8(3)	C3A	C4	C5	C6	0.1(8)
Mn1	N1	C2	C3	-4.1(6)	C4	C5	C6	C7	-0.8(8)
C27	N1	C2	C1	-60.7(6)	C5	C6	C7	C7A	0.7(8)
C27	N1	C2	C3	118.3(5)	C6	C7	C7A	C1	179.6(5)
C28	N1	C2	C1	54.7(6)	C6	C7	C7A	C3A	0.1(7)

(c) [{ κ²–(2-Me₂N-1H-inden-3-yl)P^{i}Pr₂}Mn(CO)₃(FBF₃)], molecule C

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
F1	Mn1	P1	C3	-85.8(7)	C13	Mn1	P1	C21	-151.3(12)
F1	Mn1	P1	C21	30.3(11)	C13	Mn1	P1	C24	-20.3(11)
F1	Mn1	P1	C24	161.3(10)	P1	Mn1	F1	B1	-155.2(13)
N1	Mn1	P1	C3	-0.4(7)	N1	Mn1	F1	B1	122.0(13)
N1	Mn1	P1	C21	115.7(12)	C11	Mn1	F1	B1	29.5(13)
N1	Mn1	P1	C24	-113.3(10)	C12	Mn1	F1	B1	-60.3(13)
C11	Mn1	P1	C3	24(8)	C13	Mn1	F1	B1	161(15)
C11	Mn1	P1	C21	140(7)	P1	Mn1	N1	C2	6.4(8)
C11	Mn1	P1	C24	-89(8)	P1	Mn1	N1	C27	-111.5(9)
C12	Mn1	P1	C3	-177.3(8)	P1	Mn1	N1	C28	133.2(10)
C12	Mn1	P1	C21	-61.2(12)	F1	Mn1	N1	C2	94.4(7)
C12	Mn1	P1	C24	69.8(11)	F1	Mn1	N1	C27	-23.5(8)
C13	Mn1	P1	C3	92.6(8)	F1	Mn1	N1	C28	-138.8(9)

Table 5b. Torsional Angles for **5a**•0.5C_7H_8. (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C11	Mn1	N1	C2	-171.5(8)	N1’	Mn1’	F1’	B1’	111.8(14)
C11	Mn1	N1	C27	70.6(9)	C11’	Mn1’	F1’	B1’	19.4(14)
C11	Mn1	N1	C28	-44.7(10)	C12’	Mn1’	F1’	B1’	-67.9(14)
C12	Mn1	N1	C2	58(9)	C13’	Mn1’	F1’	B1’	-70(11)
C12	Mn1	N1	C27	-60(9)	P1’	Mn1’	N1’	C2	11.4(10)
C12	Mn1	N1	C28	-175(100)	P1’	Mn1’	N1’	C27’	-111.5(13)
C13	Mn1	N1	C2	-84.1(9)	P1’	Mn1’	N1’	C28’	129.4(12)
C13	Mn1	N1	C27	158.0(9)	F1’	Mn1’	N1’	C2	97.9(9)
C13	Mn1	N1	C28	42.7(10)	F1’	Mn1’	N1’	C27’	-25.1(12)
P1	Mn1	C11	O11	92(17)	F1’	Mn1’	N1’	C28’	-144.2(11)
F1	Mn1	C11	O11	-159(15)	C11’	Mn1’	N1’	C2	-169.1(10)
N1	Mn1	C11	O11	116(15)	C11’	Mn1’	N1’	C27’	67.9(13)
C12	Mn1	C11	O11	-67(15)	C11’	Mn1’	N1’	C28’	-51.2(12)
C13	Mn1	C11	O11	23(15)	C12’	Mn1’	N1’	C2	118(75)
P1	Mn1	C12	O12	-102(18)	C12’	Mn1’	N1’	C27’	-5(76)
F1	Mn1	C12	O12	170(100)	C12’	Mn1’	N1’	C28’	-124(100)
N1	Mn1	C12	O12	-154(14)	C13’	Mn1’	N1’	C2	-82.0(10)
C11	Mn1	C12	O12	76(18)	C13’	Mn1’	N1’	C27’	155.0(13)
C13	Mn1	C12	O12	-11(18)	C13’	Mn1’	N1’	C28’	35.9(12)
P1	Mn1	C13	O13	134(20)	P1’	Mn1’	C11’	O11’	125(26)
F1	Mn1	C13	O13	178(100)	F1’	Mn1’	C11’	O11’	-166(15)
N1	Mn1	C13	O13	-143(20)	N1’	Mn1’	C11’	O11’	105(15)
C11	Mn1	C13	O13	-50(20)	C12’	Mn1’	C11’	O11’	-76(15)
C12	Mn1	C13	O13	39(20)	C13’	Mn1’	C11’	O11’	11(15)
F1’	Mn1’	P1’	C3	-97.0(7)	P1’	Mn1’	C12’	O12’	-35(21)
F1’	Mn1’	P1’	C21’	16.4(11)	F1’	Mn1’	C12’	O12’	-121(21)
F1’	Mn1’	P1’	C24’	150.3(11)	N1’	Mn1’	C12’	O12’	-141(69)
N1’	Mn1’	P1’	C3	-8.0(8)	C11’	Mn1’	C12’	O12’	146(21)
N1’	Mn1’	P1’	C21’	105.4(12)	C13’	Mn1’	C12’	O12’	58(21)
N1’	Mn1’	P1’	C24’	-120.7(11)	P1’	Mn1’	C13’	O13’	133(74)
C11’	Mn1’	P1’	C3	-28(27)	F1’	Mn1’	C13’	O13’	40(81)
C11’	Mn1’	P1’	C21’	85(27)	N1’	Mn1’	C13’	O13’	-141(100)
C11’	Mn1’	P1’	C24’	-141(26)	C11’	Mn1’	C13’	O13’	-49(74)
C12’	Mn1’	P1’	C3	172.7(8)	C12’	Mn1’	C13’	O13’	39(74)
C12’	Mn1’	P1’	C21’	-73.8(12)	Mn1	P1	C3	C2	-6.3(9)
C12’	Mn1’	P1’	C24’	60.0(12)	Mn1	P1	C3	C3A	178.1(5)
C13’	Mn1’	P1’	C3	86.2(8)	C21	P1	C3	C2	-133.6(7)
C13’	Mn1’	P1’	C21’	-160.3(11)	C21	P1	C3	C3A	50.9(14)
C13’	Mn1’	P1’	C24’	-26.5(12)	C24	P1	C3	C2	113.1(7)
P1’	Mn1’	F1’	B1’	-162.2(14)	C24	P1	C3	C3A	-62.5(11)

Table 5b. Torsional Angles for **5a**•$0.5C_7H_8$. (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
Mn1	P1	C21	C22	47.2(15)	C27	N1	C2	C3	102.7(10)
Mn1	P1	C21	C23	-74.9(13)	C28	N1	C2	C1	48.5(12)
C3	P1	C21	C22	162.6(10)	C28	N1	C2	C3	-138.9(9)
C3	P1	C21	C23	40.4(12)	Mn1’	N1’	C2	C1	168.7(6)
C24	P1	C21	C22	-86.3(13)	Mn1’	N1’	C2	C3	-11.0(12)
C24	P1	C21	C23	151.6(10)	C27’	N1’	C2	C1	-63.6(15)
Mn1	P1	C24	C25	163.3(11)	C27’	N1’	C2	C3	116.7(12)
Mn1	P1	C24	C26	-67.7(13)	C28’	N1’	C2	C1	45.4(14)
C3	P1	C24	C25	51.4(13)	C28’	N1’	C2	C3	-134.3(9)
C3	P1	C24	C26	-179.5(9)	C7A	C1	C2	N1	168.8(7)
C21	P1	C24	C25	-59.5(15)	C7A	C1	C2	N1’	175.4(9)
C21	P1	C24	C26	69.5(13)	C7A	C1	C2	C3	-4.9(6)
Mn1’	P1’	C3	C2	5.7(10)	C2	C1	C7A	C3A	3.4(6)
Mn1’	P1’	C3	C3A	-176.2(5)	C2	C1	C7A	C7	-174.7(7)
C21’	P1’	C3	C2	-117.1(7)	N1	C2	C3	P1	14.6(11)
C21’	P1’	C3	C3A	61.0(12)	N1	C2	C3	C3A	-168.5(8)
C24’	P1’	C3	C2	130.7(7)	N1’	C2	C3	P1’	2.7(12)
C24’	P1’	C3	C3A	-51.2(10)	N1’	C2	C3	C3A	-175.7(8)
Mn1’	P1’	C21’	C22’	54.5(15)	C1	C2	C3	P1	-172.3(7)
Mn1’	P1’	C21’	C23’	-74.6(14)	C1	C2	C3	P1’	-177.0(8)
C3	P1’	C21’	C22’	161.3(10)	C1	C2	C3	C3A	4.6(6)
C3	P1’	C21’	C23’	32.3(13)	P1	C3	C3A	C4	-7.7(12)
C24’	P1’	C21’	C22’	-85.9(12)	P1	C3	C3A	C7A	173.5(9)
C24’	P1’	C21’	C23’	145.0(10)	P1’	C3	C3A	C4	-1.7(11)
Mn1’	P1’	C24’	C25’	71.1(13)	P1’	C3	C3A	C7A	179.5(8)
Mn1’	P1’	C24’	C26’	-57.0(14)	C2	C3	C3A	C4	176.6(6)
C3	P1’	C24’	C25’	-36.0(10)	C2	C3	C3A	C7A	-2.2(6)
C3	P1’	C24’	C26’	-164.1(9)	C3	C3A	C4	C5	-176.6(5)
C21’	P1’	C24’	C25’	-149.7(10)	C7A	C3A	C4	C5	2.1(8)
C21’	P1’	C24’	C26’	82.2(12)	C3	C3A	C7A	C1	-1.0(6)
Mn1	F1	B1	F2	-56(2)	C3	C3A	C7A	C7	177.3(6)
Mn1	F1	B1	F3	-179.0(8)	C4	C3A	C7A	C1	-180.0(5)
Mn1	F1	B1	F4	68.2(16)	C4	C3A	C7A	C7	-1.7(9)
Mn1’	F1’	B1’	F2’	-38(2)	C3A	C4	C5	C6	-1.2(9)
Mn1’	F1’	B1’	F3’	-172.8(10)	C4	C5	C6	C7	-0.1(11)
Mn1’	F1’	B1’	F4’	68.3(17)	C5	C6	C7	C7A	0.5(11)
Mn1	N1	C2	C1	172.6(5)	C6	C7	C7A	C1	178.3(7)
Mn1	N1	C2	C3	-14.8(11)	C6	C7	C7A	C3A	0.4(10)
C27	N1	C2	C1	-69.9(11)					

Table 5b. Torsional Angles for **5a**•0.5C_7H_8. (continued)

(d) within the solvent toluene molecules

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C10S	C11S	C12S	C13S	179.3(6)	C20S	C21S	C22S	C23S	-178.0(11)
C16S	C11S	C12S	C13S	-1.3(9)	C26S	C21S	C22S	C23S	0.0†
C10S	C11S	C16S	C15S	-178.4(6)	C20S	C21S	C26S	C25S	178.0(11)
C12S	C11S	C16S	C15S	2.2(9)	C22S	C21S	C26S	C25S	0.0†
C11S	C12S	C13S	C14S	-0.6(11)	C21S	C22S	C23S	C24S	0.0†
C12S	C13S	C14S	C15S	1.5(12)	C22S	C23S	C24S	C25S	0.0†
C13S	C14S	C15S	C16S	-0.6(12)	C23S	C24S	C25S	C26S	0.0†
C14S	C15S	C16S	C11S	-1.3(11)	C24S	C25S	C26S	C21S	0.0†

†Angle fixed during refinement.

Table 6b. Least-Squares Planes for **5a**•$0.5C_7H_8$.

(a) [{κ²–(2-Me₂N-1H-inden-3-yl)P^{i}Pr₂}Mn(CO)₃(FBF₃)], molecule A

Plane	Coefficients[a]				Defining Atoms with Deviations (Å)[b]			
1	-5.624(8)	-7.82(2)	34.47(5)	8.868(8)				
					C1	-0.040(4)	C2	0.079(3)
					C3	0.003(3)	C3A	-0.045(4)
					C4	-0.020(4)	C5	0.016(4)
					C6	0.042(4)	C7	0.005(4)
					C7A	-0.040(4)		
					P1	0.022(5)	N1	0.317(5)

(b) [{κ²–(2-Me₂N-1H-inden-3-yl)P^{i}Pr₂}Mn(CO)₃(FBF₃)], molecule B

Plane	Coefficients[a]				Defining Atoms with Deviations (Å)[b]			
2	-6.243(7)	-6.06(2)	34.50(5)	5.040(9)				
					C1	0.018(4)	C2	-0.023(4)
					C3	-0.005(4)	C3A	0.009(4)
					C4	0.010(4)	C5	-0.001(4)
					C6	-0.016(4)	C7	-0.003(4)
					C7A	0.010(4)		
					P1	0.005(5)	N1	-0.091(6)

(c) [{κ²–(2-Me₂N-1H-inden-3-yl)P^{i}Pr₂}Mn(CO)₃(FBF₃)], molecule C

Plane	Coefficients[a]				Defining Atoms with Deviations (Å)[b]			
3	6.061(10)	-7.18(2)	-32.52(6)	1.565(12)				
					C1	0.032(5)	C2	-0.060(4)
					C3	-0.001(4)	C3A	0.026(5)
					C4	0.024(5)	C5	-0.017(5)
					C6	-0.031(6)	C7	-0.003(6)
					C7A	0.031(6)		
					P1	0.115(18)	N1	-0.333(14)
					P1’	0.00(2)	N1’	-0.191(16)

[a]Coefficients are for the form $ax+by+cz = d$ where x, y and z are crystallographic coordinates.
[b]Underlined atoms were not included in the definition of the plane.

Table 7b. Anisotropic Displacement Parameters (U_{ij}, Å^2) for **5a**•0.5C_7H_8.

(a) [{κ²–(2-Me$_2$N-1H-inden-3-yl)P^{i}Pr$_2$}Mn(CO)$_3$(FBF$_3$)], molecule A

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mn1	0.0266(3)	0.0291(4)	0.0223(3)	0.0022(3)	-0.0017(3)	-0.0035(3)
P1	0.0193(5)	0.0220(5)	0.0222(5)	0.0020(4)	-0.0005(4)	0.0025(4)
F1	0.0483(17)	0.0383(16)	0.0307(14)	0.0022(12)	0.0066(12)	-0.0158(13)
F2	0.130(5)	0.198(6)	0.091(4)	0.010(4)	0.052(3)	-0.092(5)
F3	0.160(4)	0.068(3)	0.0322(18)	0.0009(17)	0.008(2)	-0.049(3)
F4	0.276(8)	0.045(3)	0.069(3)	0.021(2)	0.040(4)	0.012(4)
O11	0.077(3)	0.076(3)	0.034(2)	-0.013(2)	0.000(2)	-0.040(2)
O12	0.069(3)	0.080(3)	0.059(3)	0.016(2)	-0.022(2)	0.033(3)
O13	0.033(2)	0.066(3)	0.048(2)	-0.0027(19)	0.0044(17)	-0.0178(19)
N1	0.0266(19)	0.025(2)	0.0257(19)	-0.0045(15)	0.0070(15)	-0.0025(15)
C1	0.029(2)	0.026(2)	0.040(3)	0.005(2)	0.004(2)	0.0067(19)
C2	0.018(2)	0.025(2)	0.029(2)	0.0047(18)	0.0042(17)	0.0010(17)
C3	0.020(2)	0.022(2)	0.0210(19)	0.0023(17)	-0.0003(15)	-0.0019(16)
C3A	0.022(2)	0.027(2)	0.026(2)	0.0063(18)	-0.0001(16)	-0.0008(18)
C4	0.035(3)	0.035(3)	0.032(2)	0.002(2)	-0.001(2)	-0.002(2)
C5	0.044(3)	0.045(3)	0.029(2)	0.001(2)	-0.007(2)	-0.012(2)
C6	0.033(3)	0.058(4)	0.038(3)	0.018(3)	-0.012(2)	-0.012(2)
C7	0.026(2)	0.040(3)	0.045(3)	0.018(2)	-0.005(2)	0.001(2)
C7A	0.022(2)	0.027(2)	0.035(2)	0.0113(19)	0.0014(18)	0.0014(18)
C11	0.043(3)	0.043(3)	0.038(3)	0.000(2)	0.005(2)	-0.018(2)
C12	0.046(3)	0.050(3)	0.031(3)	0.003(2)	-0.008(2)	0.002(3)
C13	0.024(2)	0.038(3)	0.031(2)	0.000(2)	-0.0044(19)	-0.004(2)
C21	0.033(2)	0.022(2)	0.030(2)	-0.0043(18)	0.0018(18)	0.0018(19)
C22	0.047(3)	0.028(3)	0.055(3)	0.008(2)	0.004(3)	0.011(2)
C23	0.035(3)	0.033(3)	0.045(3)	0.002(2)	0.004(2)	-0.005(2)
C24	0.024(2)	0.033(3)	0.029(2)	0.0006(19)	0.0060(18)	0.0016(18)
C25	0.029(3)	0.065(4)	0.056(3)	0.011(3)	0.015(2)	0.014(3)
C26	0.041(3)	0.061(4)	0.039(3)	-0.014(3)	0.016(2)	-0.011(3)
C27	0.036(3)	0.054(3)	0.032(3)	-0.006(2)	0.011(2)	0.003(2)
C28	0.050(3)	0.025(3)	0.044(3)	-0.006(2)	-0.002(2)	-0.002(2)
B1	0.098(6)	0.042(4)	0.041(4)	0.000(3)	0.026(4)	-0.025(4)

(b) [{κ²–(2-Me$_2$N-1H-inden-3-yl)P^{i}Pr$_2$}Mn(CO)$_3$(FBF$_3$)], molecule B

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mn1	0.0387(4)	0.0302(4)	0.0350(4)	0.0047(3)	-0.0128(3)	-0.0065(3)
P1	0.0258(6)	0.0219(6)	0.0286(6)	0.0001(5)	-0.0017(4)	0.0009(5)
F1	0.064(2)	0.0432(18)	0.0334(15)	0.0018(13)	0.0012(14)	-0.0186(15)
F2	0.228(7)	0.063(3)	0.067(3)	0.026(2)	-0.006(3)	-0.018(4)
F3	0.263(7)	0.098(4)	0.040(2)	-0.011(2)	0.000(3)	-0.089(4)

Table 7b. Anisotropic Displacement Parameters for **5a**•0.5C_7H_8. (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
F4	0.137(5)	0.178(6)	0.096(4)	0.014(4)	0.066(4)	-0.027(5)
O11	0.142(5)	0.092(4)	0.060(3)	0.006(3)	-0.053(3)	-0.052(4)
O12	0.089(4)	0.079(4)	0.124(5)	0.020(3)	-0.042(3)	0.035(3)
O13	0.059(3)	0.116(5)	0.094(4)	-0.008(3)	0.007(3)	-0.048(3)
N1	0.054(3)	0.026(2)	0.0220(19)	-0.0018(16)	-0.0043(18)	-0.0033(18)
C1	0.039(3)	0.027(2)	0.041(3)	0.002(2)	0.008(2)	0.004(2)
C2	0.034(2)	0.025(2)	0.026(2)	0.0025(18)	0.0036(19)	-0.0018(19)
C3	0.029(2)	0.027(2)	0.020(2)	0.0011(17)	0.0013(17)	-0.0009(18)
C3A	0.027(2)	0.034(3)	0.027(2)	0.0068(19)	0.0020(18)	0.0012(19)
C4	0.045(3)	0.044(3)	0.027(2)	0.001(2)	-0.004(2)	-0.001(2)
C5	0.050(3)	0.075(4)	0.023(2)	0.005(3)	-0.007(2)	-0.013(3)
C6	0.038(3)	0.073(4)	0.039(3)	0.028(3)	-0.008(2)	-0.001(3)
C7	0.033(3)	0.050(3)	0.045(3)	0.021(3)	0.002(2)	0.005(2)
C7A	0.026(2)	0.035(3)	0.035(3)	0.011(2)	0.0027(19)	-0.0015(19)
C11	0.073(4)	0.051(4)	0.051(4)	0.013(3)	-0.030(3)	-0.027(3)
C12	0.056(4)	0.055(4)	0.057(4)	0.009(3)	-0.023(3)	0.004(3)
C13	0.053(4)	0.057(4)	0.056(4)	0.001(3)	-0.016(3)	-0.018(3)
C21	0.046(3)	0.028(2)	0.028(2)	-0.002(2)	-0.002(2)	-0.008(2)
C22	0.068(4)	0.025(3)	0.049(3)	0.006(2)	-0.005(3)	-0.003(3)
C23	0.044(3)	0.050(3)	0.050(3)	0.005(3)	-0.002(3)	-0.016(3)
C24	0.036(3)	0.038(3)	0.047(3)	-0.014(2)	0.010(2)	-0.002(2)
C25	0.054(4)	0.060(4)	0.099(6)	-0.001(4)	0.033(4)	0.020(3)
C26	0.051(3)	0.057(4)	0.051(3)	-0.002(3)	0.020(3)	-0.006(3)
C27	0.108(6)	0.069(5)	0.035(3)	-0.010(3)	0.012(3)	0.035(4)
C28	0.107(6)	0.029(3)	0.068(4)	0.004(3)	-0.046(4)	-0.020(3)
B1	0.123(8)	0.056(5)	0.036(4)	-0.003(3)	0.022(4)	-0.040(5)

(c) [{κ²–(2-Me₂N-1H-inden-3-yl)P^{i}Pr₂}Mn(CO)₃(FBF₃)], molecule C

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mn1	0.0323(15)	0.0359(15)	0.032(2)	-0.0006(17)	-0.0096(15)	-0.0011(10)
Mn1’	0.050(3)	0.038(2)	0.033(2)	-0.0062(17)	-0.0119(16)	0.0128(18)
P1	0.033(5)	0.032(6)	0.028(4)	-0.004(3)	0.002(3)	-0.007(3)
P1’	0.027(2)	0.026(5)	0.037(5)	-0.001(3)	-0.007(3)	-0.001(3)
C1	0.051(3)	0.052(4)	0.046(3)	-0.003(3)	0.002(3)	-0.022(3)
C2	0.033(3)	0.038(3)	0.033(3)	-0.008(2)	0.001(2)	-0.001(2)
C3	0.029(2)	0.039(3)	0.032(2)	-0.008(2)	0.0022(19)	-0.009(2)
C3A	0.034(3)	0.050(3)	0.028(2)	-0.010(2)	0.002(2)	-0.008(2)
C4	0.047(3)	0.059(4)	0.034(3)	-0.002(3)	-0.001(2)	-0.001(3)
C5	0.056(4)	0.084(5)	0.037(3)	-0.002(3)	-0.005(3)	0.005(3)
C6	0.054(4)	0.125(7)	0.042(4)	-0.011(4)	-0.013(3)	-0.019(4)

Table 7b. Anisotropic Displacement Parameters for **5a**•0.5C_7H_8. (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C7	0.054(4)	0.105(6)	0.044(4)	-0.011(4)	-0.008(3)	-0.040(4)
C7A	0.043(3)	0.065(4)	0.042(3)	-0.008(3)	-0.001(2)	-0.018(3)

(d) solvent toluene atoms

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C10S	0.111(7)	0.084(6)	0.090(6)	-0.026(5)	-0.024(5)	-0.003(5)
C11S	0.076(5)	0.055(4)	0.049(4)	-0.026(3)	0.002(3)	-0.013(3)
C12S	0.115(7)	0.051(4)	0.064(5)	-0.027(3)	0.020(5)	-0.024(4)
C13S	0.100(7)	0.096(7)	0.100(7)	-0.065(6)	0.025(6)	-0.035(6)
C14S	0.080(6)	0.132(10)	0.120(9)	-0.092(8)	-0.029(6)	0.030(6)
C15S	0.131(9)	0.084(6)	0.072(6)	-0.043(5)	-0.025(6)	0.033(6)
C16S	0.113(7)	0.054(4)	0.047(4)	-0.019(3)	0.007(4)	-0.016(4)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table 8b. Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms for **5a**•0.5C_7H_8.

(a) [{κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}Mn(CO)$_3$(FBF_3)], molecule A

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1A	-0.3902	-0.0216	0.2098	0.038
H1B	-0.2499	0.0272	0.1971	0.038
H4	-0.1770	-0.2720	0.1659	0.041
H5	-0.3811	-0.2531	0.1383	0.048
H6	-0.5573	-0.1338	0.1385	0.052
H7	-0.5266	-0.0278	0.1653	0.045
H21	-0.0305	-0.3585	0.1966	0.034
H22A	0.1806	-0.3961	0.2229	0.052
H22B	0.0276	-0.4607	0.2241	0.052
H22C	0.0561	-0.3840	0.2415	0.052
H23A	-0.2836	-0.3038	0.2079	0.045
H23B	-0.2286	-0.3276	0.2324	0.045
H23C	-0.2576	-0.4041	0.2149	0.045
H24	0.2336	-0.1521	0.1937	0.034
H25A	0.3928	-0.2388	0.2185	0.059
H25B	0.4563	-0.2439	0.1947	0.059
H25C	0.3529	-0.3232	0.2038	0.059
H26A	0.0645	-0.2197	0.1663	0.056
H26B	0.1534	-0.3112	0.1717	0.056
H26C	0.2550	-0.2311	0.1626	0.056
H27A	-0.2051	-0.0569	0.2644	0.048
H27B	-0.2891	-0.1294	0.2487	0.048
H27C	-0.3265	-0.0275	0.2446	0.048
H28A	0.0008	0.0432	0.2506	0.048
H28B	-0.1336	0.0681	0.2319	0.048
H28C	0.0443	0.0364	0.2259	0.048

(b) [{κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}Mn(CO)$_3$(FBF_3)], molecule B

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1A	-0.1477	-0.0584	0.1334	0.042
H1B	-0.0007	-0.0189	0.1201	0.042
H4	-0.0904	0.2318	0.1710	0.047
H5	0.1067	0.1796	0.1970	0.060
H6	0.2243	0.0430	0.1932	0.060
H7	0.1454	-0.0468	0.1640	0.051
H21	-0.1867	0.3473	0.1402	0.041
H22A	-0.3930	0.4117	0.1172	0.057
H22B	-0.2985	0.3818	0.0966	0.057
H22C	-0.2178	0.4525	0.1130	0.057

Table 8b. Derived Parameters for Hydrogen Atoms for **5a**•0.5C_7H_8. (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H23A	0.0188	0.2597	0.1259	0.058
H23B	0.0346	0.3601	0.1188	0.058
H23C	-0.0424	0.2896	0.1020	0.058
H24	-0.3794	0.2758	0.1607	0.048
H25A	-0.5631	0.3606	0.1384	0.084
H25B	-0.6528	0.3191	0.1582	0.084
H25C	-0.6789	0.2767	0.1346	0.084
H26A	-0.4124	0.1224	0.1627	0.063
H26B	-0.5860	0.1304	0.1496	0.063
H26C	-0.5597	0.1728	0.1731	0.063
H27A	-0.2359	0.0413	0.0688	0.085
H27B	-0.1113	-0.0064	0.0858	0.085
H27C	-0.1037	0.0978	0.0828	0.085
H28A	-0.4592	-0.0311	0.0871	0.084
H28B	-0.4680	-0.0205	0.1126	0.084
H28C	-0.3212	-0.0744	0.1030	0.084

(c) [{κ^2–(2-Me_2N-1H-inden-3-yl)P^iPr_2}Mn(CO)$_3$(FBF_3)], molecule C

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1A	-0.0895	-0.5351	0.0267	0.060
H1B	-0.2376	-0.4898	0.0387	0.060
H4	-0.0398	-0.2351	-0.0052	0.056
H5	-0.2365	-0.2607	-0.0335	0.071
H6	-0.3921	-0.3865	-0.0340	0.089
H7	-0.3603	-0.4901	-0.0069	0.082
H21[a]	0.1126	-0.1451	0.0278	0.042
H22A[a]	0.3162	-0.1085	0.0553	0.057
H22B[a]	0.1918	-0.1294	0.0735	0.057
H22C[a]	0.1590	-0.0477	0.0576	0.057
H23A[a]	-0.1443	-0.2006	0.0372	0.046
H23B[a]	-0.1193	-0.1028	0.0462	0.046
H23C[a]	-0.0944	-0.1845	0.0622	0.046
H24[a]	0.3804	-0.3556	0.0264	0.064
H25A[a]	0.2389	-0.3198	-0.0028	0.072
H25B[a]	0.4100	-0.2701	-0.0041	0.072
H25C[a]	0.2513	-0.2171	0.0023	0.072
H26A[a]	0.4684	-0.1927	0.0431	0.075
H26B[a]	0.5560	-0.2188	0.0216	0.075
H26C[a]	0.5741	-0.2809	0.0424	0.075
H27A[a]	-0.0810	-0.4375	0.0938	0.037

Table 8b. Derived Parameters for Hydrogen Atoms for **5a**•0.5C_7H_8. (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H27B[a]	-0.2034	-0.4617	0.0737	0.037
H27C[a]	-0.1452	-0.3624	0.0774	0.037
H28A[a]	0.1118	-0.5411	0.0841	0.043
H28B[a]	0.1740	-0.5455	0.0601	0.043
H28C[a]	-0.0110	-0.5706	0.0644	0.043
H21'[a]	0.0420	-0.1334	0.0296	0.039
H22A'[a]	0.2567	-0.0894	0.0533	0.059
H22B'[a]	0.1582	-0.1208	0.0734	0.059
H22C'[a]	0.0911	-0.0408	0.0587	0.059
H23A'[a]	-0.1800	-0.2113	0.0401	0.054
H23B'[a]	-0.1756	-0.1164	0.0511	0.054
H23C'[a]	-0.1194	-0.2009	0.0649	0.054
H24'[a]	0.2379	-0.2061	0.0084	0.043
H25A'[a]	0.2338	-0.3461	-0.0035	0.052
H25B'[a]	0.3544	-0.3801	0.0159	0.052
H25C'[a]	0.4244	-0.3227	-0.0030	0.052
H26A'[a]	0.4637	-0.2018	0.0421	0.075
H26B'[a]	0.4467	-0.1389	0.0214	0.075
H26C'[a]	0.5463	-0.2289	0.0203	0.075
H27A'[a]	-0.0288	-0.4387	0.0941	0.085
H27B'[a]	-0.1519	-0.4783	0.0756	0.085
H27C'[a]	-0.1325	-0.3743	0.0782	0.085
H28A'[a]	0.1706	-0.5427	0.0779	0.079
H28B'[a]	0.1902	-0.5367	0.0525	0.079
H28C'[a]	0.0193	-0.5661	0.0614	0.079

(d) solvent toluene hydrogens

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H10A	-0.4528	-0.4058	0.1742	0.116
H10B	-0.5189	-0.5022	0.1683	0.116
H10C	-0.4622	-0.4386	0.1497	0.116
H12S	-0.1766	-0.4159	0.1450	0.091
H13S	0.0851	-0.4689	0.1498	0.117
H14S	0.1535	-0.5738	0.1757	0.134
H15S	-0.0556	-0.6310	0.1965	0.116
H16S	-0.3215	-0.5798	0.1909	0.086
H20A[a]	0.3226	-0.0767	-0.0157	0.089
H20B[a]	0.3851	0.0044	-0.0011	0.089
H20C[a]	0.3138	0.0207	-0.0253	0.089
H22S[a]	0.0169	-0.0866	-0.0261	0.089

Table 8b. Derived Parameters for Hydrogen Atoms for **5a**•0.5C_7H_8. (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H23S[a]	-0.2470	-0.0664	-0.0145	0.089
H24S[a]	-0.2898	0.0283	0.0143	0.089
H25S[a]	-0.0687	0.1027	0.0315	0.089
H26S[a]	0.1952	0.0826	0.0199	0.089

[a]Refined with an occupancy factor of 0.5.

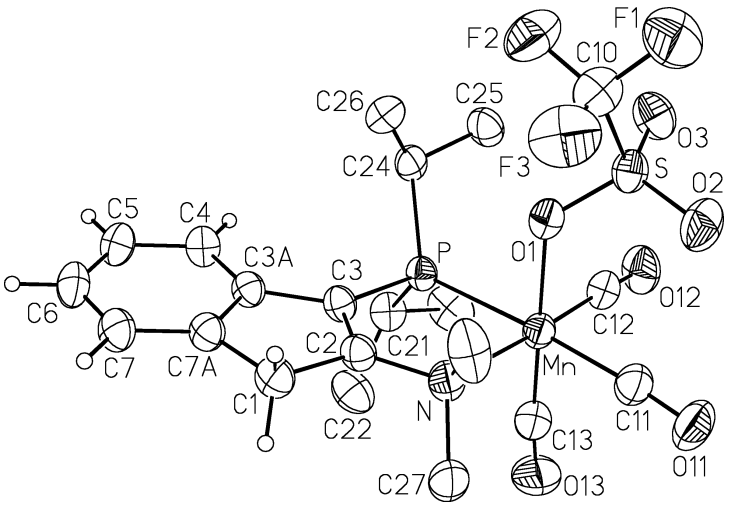

Figure 1c. Perspective view of the [{κ^2–(2-Me$_2$N-1*H*-inden-3-yl)P^{i}Pr$_2$}Mn(CO)$_3$(OSO$_2$-CF$_3$)] molecule showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 20% probability level. Hydrogen atoms of the indenyl group are shown with arbitrarily small thermal parameters; methyl and isopropyl hydrogens are not shown.

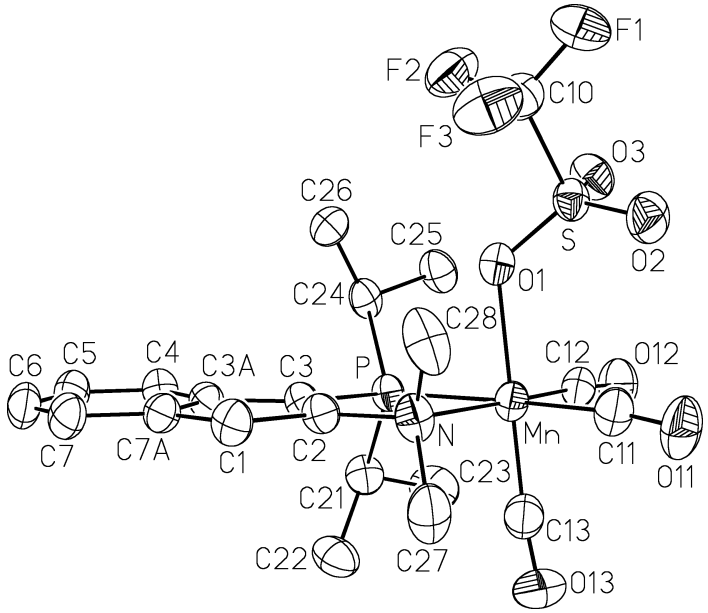

Figure 2c. Alternative view of the molecule, with the indenyl group oriented nearly edge-on. Hydrogen atoms are not shown.

Table 1c. Crystallographic Experimental Details for **5b**.

A. Crystal Data	
formula	$C_{21}H_{26}F_3MnNO_6PS$
formula weight	563.40
crystal dimensions (mm)	$0.29 \times 0.22 \times 0.20$
crystal system	monoclinic
space group	$P2_1/n$ (an alternate setting of $P2_1/c$ [No. 14])
unit cell parameters[a]	
a (Å)	11.9460 (5)
b (Å)	14.3629 (6)
c (Å)	14.5832 (6)
β (deg)	96.9755 (8)
V (Å^3)	2483.65 (18)
Z	4
ρ_{calcd} (g cm^{-3})	1.507
μ (mm^{-1})	0.739
B. Data Collection and Refinement Conditions	
diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.2°) (20 s exposures)
data collection 2θ limit (deg)	52.74
total data collected	15849 ($-14 \le h \le 14$, $-17 \le k \le 17$, $-18 \le l \le 18$)
independent reflections	5053 (R_{int} = 0.0310)
number of observed reflections (*NO*)	4230 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–86*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	multi-scan (*SADABS*)
range of transmission factors	0.8663–0.8142
data/restraints/parameters	5053 [$F_o^2 \ge -3\sigma(F_o^2)$] / 0 / 307
goodness-of-fit (S)[e]	1.045 [$F_o^2 \ge -3\sigma(F_o^2)$]
final R indices[f]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0379
wR_2 [$F_o^2 \ge -3\sigma(F_o^2)$]	0.0937
largest difference peak and hole	0.428 and –0.182 e Å^{-3}

[a]Obtained from least-squares refinement of 7535 reflections with $4.45° < 2\theta < 52.65°$.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table 1c. Crystallographic Experimental Details for **5b**. (continued)

[c]Sheldrick, G. M. *Acta Crystallogr.* **1990**, *A46*, 467–473.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted *R*-factors wR_2 and all goodnesses of fit *S* are based on F_o^2; conventional *R*-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. *R*-factors based on F_o^2 are statistically about twice as large as those based on F_o, and *R*-factors based on ALL data will be even larger.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0484P)^2 + 0.8196P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2c. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for **5b**.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Mn	0.21804(3)	0.37394(2)	0.06421(2)	0.03276(10)*
S	0.42160(5)	0.44548(4)	0.20550(4)	0.03568(14)*
P	0.19943(4)	0.21678(4)	0.10235(4)	0.02920(13)*
F1	0.62732(14)	0.47795(13)	0.27816(14)	0.0769(5)*
F2	0.58772(13)	0.33325(12)	0.26585(12)	0.0668(4)*
F3	0.61571(13)	0.41139(15)	0.14587(12)	0.0745(5)*
O1	0.37612(12)	0.37044(10)	0.14379(10)	0.0359(3)*
O2	0.42084(15)	0.53532(12)	0.16297(13)	0.0526(4)*
O3	0.38623(14)	0.44190(12)	0.29519(11)	0.0479(4)*
O11	0.23576(18)	0.56986(12)	-0.00155(13)	0.0599(5)*
O12	0.09239(16)	0.43576(13)	0.21516(12)	0.0550(5)*
O13	-0.00225(17)	0.38728(15)	-0.04644(14)	0.0670(6)*
N	0.30790(17)	0.31961(13)	-0.04829(12)	0.0381(4)*
C1	0.37443(19)	0.16245(16)	-0.11483(15)	0.0379(5)*
C2	0.31639(18)	0.21890(15)	-0.04655(14)	0.0323(4)*
C3	0.27500(17)	0.16407(14)	0.01579(13)	0.0305(4)*
C3A	0.30087(17)	0.06602(14)	-0.00422(14)	0.0311(4)*
C4	0.27821(18)	-0.01627(15)	0.03945(15)	0.0363(5)*
C5	0.31308(19)	-0.09967(16)	0.00359(17)	0.0413(5)*
C6	0.3689(2)	-0.10054(17)	-0.07438(17)	0.0442(6)*
C7	0.39306(19)	-0.01815(17)	-0.11744(16)	0.0408(5)*
C7A	0.35892(17)	0.06475(15)	-0.08224(14)	0.0335(5)*
C10	0.5705(2)	0.41509(19)	0.22439(19)	0.0497(6)*
C11	0.2359(2)	0.49584(17)	0.02575(16)	0.0430(5)*
C12	0.1446(2)	0.41196(16)	0.15870(16)	0.0391(5)*
C13	0.0846(2)	0.37758(17)	-0.00484(17)	0.0465(6)*
C21	0.05988(18)	0.15792(17)	0.08737(16)	0.0395(5)*
C22	0.0139(2)	0.1440(2)	-0.01338(18)	0.0533(7)*
C23	-0.0262(2)	0.2077(2)	0.1401(2)	0.0599(8)*
C24	0.26610(19)	0.17029(15)	0.21462(14)	0.0353(5)*
C25	0.2378(2)	0.22877(17)	0.29656(15)	0.0450(6)*
C26	0.3934(2)	0.15845(18)	0.21686(17)	0.0451(6)*
C27	0.2469(3)	0.34806(19)	-0.14032(16)	0.0573(7)*
C28	0.4247(2)	0.35793(18)	-0.04255(19)	0.0553(7)*

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$.

Table 3c. Selected Interatomic Distances (Å) for **5b**.

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Mn	P	2.3419(6)	O13	C13	1.146(3)
Mn	O1	2.0935(15)	N	C2	1.450(3)
Mn	N	2.2091(17)	N	C27	1.504(3)
Mn	C11	1.859(2)	N	C28	1.493(3)
Mn	C12	1.806(2)	C1	C2	1.516(3)
Mn	C13	1.779(3)	C1	C7A	1.500(3)
S	O1	1.4657(16)	C2	C3	1.342(3)
S	O2	1.4313(17)	C3	C3A	1.478(3)
S	O3	1.4234(16)	C3A	C4	1.385(3)
S	C10	1.820(3)	C3A	C7A	1.403(3)
P	C3	1.805(2)	C4	C5	1.391(3)
P	C21	1.858(2)	C5	C6	1.387(3)
P	C24	1.856(2)	C6	C7	1.386(3)
F1	C10	1.327(3)	C7	C7A	1.378(3)
F2	C10	1.326(3)	C21	C22	1.518(3)
F3	C10	1.325(3)	C21	C23	1.533(3)
O11	C11	1.135(3)	C24	C25	1.532(3)
O12	C12	1.144(3)	C24	C26	1.526(3)

Table 4c. Selected Interatomic Angles (deg) for **5b**.

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
P	Mn	O1	87.16(4)	C27	N	C28	107.3(2)
P	Mn	N	84.53(5)	C2	C1	C7A	102.02(16)
P	Mn	C11	175.83(7)	N	C2	C1	123.97(18)
P	Mn	C12	92.37(7)	N	C2	C3	124.51(18)
P	Mn	C13	93.35(8)	C1	C2	C3	111.52(19)
O1	Mn	N	85.20(7)	P	C3	C2	118.98(16)
O1	Mn	C11	93.51(9)	P	C3	C3A	132.21(15)
O1	Mn	C12	94.21(8)	C2	C3	C3A	108.80(17)
O1	Mn	C13	179.15(9)	C3	C3A	C4	131.68(18)
N	Mn	C11	91.43(8)	C3	C3A	C7A	107.95(17)
N	Mn	C12	176.86(9)	C4	C3A	C7A	120.36(19)
N	Mn	C13	94.17(9)	C3A	C4	C5	118.55(19)
C11	Mn	C12	91.69(10)	C4	C5	C6	120.8(2)
C11	Mn	C13	85.94(11)	C5	C6	C7	120.7(2)
C12	Mn	C13	86.46(11)	C6	C7	C7A	118.79(19)
O1	S	O2	114.49(10)	C1	C7A	C3A	109.70(18)
O1	S	O3	114.10(10)	C1	C7A	C7	129.54(18)
O1	S	C10	101.50(11)	C3A	C7A	C7	120.8(2)
O2	S	O3	116.35(11)	S	C10	F1	110.27(19)
O2	S	C10	103.68(11)	S	C10	F2	112.07(17)
O3	S	C10	104.25(11)	S	C10	F3	111.84(18)
Mn	P	C3	99.68(7)	F1	C10	F2	107.1(2)
Mn	P	C21	121.35(8)	F1	C10	F3	107.8(2)
Mn	P	C24	120.89(7)	F2	C10	F3	107.6(2)
C3	P	C21	104.17(10)	Mn	C11	O11	173.1(2)
C3	P	C24	105.58(10)	Mn	C12	O12	176.0(2)
C21	P	C24	102.88(10)	Mn	C13	O13	174.3(2)
Mn	O1	S	124.40(9)	P	C21	C22	112.79(16)
Mn	N	C2	112.25(12)	P	C21	C23	112.07(17)
Mn	N	C27	109.90(15)	C22	C21	C23	111.1(2)
Mn	N	C28	111.30(14)	P	C24	C25	112.28(16)
C2	N	C27	108.17(18)	P	C24	C26	112.25(15)
C2	N	C28	107.69(18)	C25	C24	C26	110.99(19)

Table 5c. Torsional Angles (deg) for **5b**.

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
O1	Mn	P	C3	-83.69(8)	P	Mn	C12	O12	-90(3)
O1	Mn	P	C21	163.06(9)	O1	Mn	C12	O12	-177(100)
O1	Mn	P	C24	31.11(9)	N	Mn	C12	O12	-98(3)
N	Mn	P	C3	1.75(9)	C11	Mn	C12	O12	89(3)
N	Mn	P	C21	-111.50(10)	C13	Mn	C12	O12	3(3)
N	Mn	P	C24	116.55(10)	P	Mn	C13	O13	142(2)
C11	Mn	P	C3	15.7(11)	O1	Mn	C13	O13	-91(7)
C11	Mn	P	C21	-97.6(11)	N	Mn	C13	O13	-133(2)
C11	Mn	P	C24	130.5(11)	C11	Mn	C13	O13	-42(2)
C12	Mn	P	C3	-177.79(10)	C12	Mn	C13	O13	50(2)
C12	Mn	P	C21	68.96(11)	O2	S	O1	Mn	-52.81(13)
C12	Mn	P	C24	-62.99(11)	O3	S	O1	Mn	84.75(13)
C13	Mn	P	C3	95.62(11)	C10	S	O1	Mn	-163.77(11)
C13	Mn	P	C21	-17.62(12)	O1	S	C10	F1	178.45(17)
C13	Mn	P	C24	-149.58(11)	O1	S	C10	F2	-62.4(2)
P	Mn	O1	S	-139.83(10)	O1	S	C10	F3	58.5(2)
N	Mn	O1	S	135.43(11)	O2	S	C10	F1	59.4(2)
C11	Mn	O1	S	44.29(12)	O2	S	C10	F2	178.65(19)
C12	Mn	O1	S	-47.66(12)	O2	S	C10	F3	-60.5(2)
C13	Mn	O1	S	94(6)	O3	S	C10	F1	-62.8(2)
P	Mn	N	C2	-1.23(14)	O3	S	C10	F2	56.4(2)
P	Mn	N	C27	119.20(16)	O3	S	C10	F3	177.32(19)
P	Mn	N	C28	-122.03(16)	Mn	P	C3	C2	-2.49(18)
O1	Mn	N	C2	86.37(15)	Mn	P	C3	C3A	179.31(19)
O1	Mn	N	C27	-153.20(16)	C21	P	C3	C2	123.48(18)
O1	Mn	N	C28	-34.43(16)	C21	P	C3	C3A	-54.7(2)
C11	Mn	N	C2	179.77(16)	C24	P	C3	C2	-128.52(18)
C11	Mn	N	C27	-59.80(18)	C24	P	C3	C3A	53.3(2)
C11	Mn	N	C28	58.98(18)	Mn	P	C21	C22	69.8(2)
C12	Mn	N	C2	7.2(18)	Mn	P	C21	C23	-56.5(2)
C12	Mn	N	C27	127.6(17)	C3	P	C21	C22	-41.1(2)
C12	Mn	N	C28	-113.6(17)	C3	P	C21	C23	-167.41(19)
C13	Mn	N	C2	-94.20(16)	C24	P	C21	C22	-151.05(18)
C13	Mn	N	C27	26.23(18)	C24	P	C21	C23	82.6(2)
C13	Mn	N	C28	145.01(18)	Mn	P	C24	C25	50.83(18)
P	Mn	C11	O11	89(2)	Mn	P	C24	C26	-75.04(17)
O1	Mn	C11	O11	-172.4(17)	C3	P	C24	C25	162.56(16)
N	Mn	C11	O11	102.4(17)	C3	P	C24	C26	36.68(18)
C12	Mn	C11	O11	-78.0(17)	C21	P	C24	C25	-88.51(17)
C13	Mn	C11	O11	8.3(17)	C21	P	C24	C26	145.61(16)

Table 5c. Torsional Angles for **5b**. (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
Mn	N	C2	C1	-179.47(17)	P	C3	C3A	C7A	177.77(17)
Mn	N	C2	C3	-0.1(3)	C2	C3	C3A	C4	179.2(2)
C27	N	C2	C1	59.1(3)	C2	C3	C3A	C7A	-0.6(2)
C27	N	C2	C3	-121.5(2)	C3	C3A	C4	C5	179.6(2)
C28	N	C2	C1	-56.6(3)	C7A	C3A	C4	C5	-0.7(3)
C28	N	C2	C3	122.8(2)	C3	C3A	C7A	C1	0.9(2)
C7A	C1	C2	N	180.0(2)	C3	C3A	C7A	C7	-179.4(2)
C7A	C1	C2	C3	0.5(2)	C4	C3A	C7A	C1	-178.87(19)
C2	C1	C7A	C3A	-0.9(2)	C4	C3A	C7A	C7	0.8(3)
C2	C1	C7A	C7	179.5(2)	C3A	C4	C5	C6	-0.2(3)
N	C2	C3	P	1.9(3)	C4	C5	C6	C7	1.1(4)
N	C2	C3	C3A	-179.47(19)	C5	C6	C7	C7A	-1.0(4)
C1	C2	C3	P	-178.60(15)	C6	C7	C7A	C1	179.7(2)
C1	C2	C3	C3A	0.0(3)	C6	C7	C7A	C3A	0.1(3)
P	C3	C3A	C4	-2.5(4)					

Table 6c. Least-Squares Planes for **5b**.

Plane	Coefficients[a]				Defining Atoms with Deviations (Å)[b]			
1	9.613(5)	0.988(7)	7.111(10)	2.929(2)				
					C1	0.0140(18)	C2	-0.0026(17)
					C3	-0.0114(17)	C3A	-0.0019(19)
					C4	0.0095(18)	C5	0.0073(19)
					C6	-0.0110(19)	C7	-0.0040(19)
					C7A	0.0001(19)		
					P	-0.070(3)	N	0.003(3)

[a]Coefficients are for the form $ax+by+cz = d$ where x, y and z are crystallographic coordinates.
[b]Underlined atoms were not included in the definition of the plane.

Table 7c. Anisotropic Displacement Parameters (U_{ij}, Å^2) for **5b**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mn	0.03892(19)	0.02839(18)	0.03171(18)	0.00095(12)	0.00723(13)	0.00356(13)
S	0.0362(3)	0.0302(3)	0.0422(3)	0.0002(2)	0.0109(2)	-0.0017(2)
P	0.0318(3)	0.0284(3)	0.0289(3)	-0.0013(2)	0.0100(2)	-0.0007(2)
F1	0.0495(9)	0.0753(12)	0.1018(14)	-0.0091(10)	-0.0081(9)	-0.0185(9)
F2	0.0520(9)	0.0607(10)	0.0858(12)	0.0174(9)	0.0005(8)	0.0097(8)
F3	0.0452(9)	0.1074(14)	0.0758(11)	0.0110(10)	0.0273(8)	0.0069(9)
O1	0.0387(8)	0.0301(8)	0.0398(8)	0.0004(6)	0.0081(7)	0.0031(6)
O2	0.0523(10)	0.0340(9)	0.0719(12)	0.0078(8)	0.0087(9)	-0.0060(8)
O3	0.0496(10)	0.0521(11)	0.0442(9)	-0.0090(8)	0.0147(8)	-0.0055(8)
O11	0.0884(15)	0.0357(10)	0.0582(11)	0.0119(8)	0.0198(10)	0.0115(9)
O12	0.0597(11)	0.0520(11)	0.0573(11)	-0.0109(8)	0.0240(9)	0.0102(9)
O13	0.0581(12)	0.0754(14)	0.0616(12)	-0.0019(10)	-0.0171(10)	0.0120(10)
N	0.0535(12)	0.0306(10)	0.0323(9)	0.0021(7)	0.0136(8)	-0.0029(8)
C1	0.0409(12)	0.0419(13)	0.0335(11)	0.0002(9)	0.0147(9)	0.0033(10)
C2	0.0347(11)	0.0336(11)	0.0296(10)	-0.0008(8)	0.0079(8)	-0.0004(9)
C3	0.0321(11)	0.0305(11)	0.0300(10)	-0.0026(8)	0.0086(8)	-0.0026(8)
C3A	0.0285(10)	0.0327(11)	0.0326(10)	-0.0031(8)	0.0059(8)	0.0002(8)
C4	0.0361(11)	0.0333(12)	0.0414(12)	-0.0018(9)	0.0129(9)	-0.0038(9)
C5	0.0420(13)	0.0302(12)	0.0527(14)	0.0003(10)	0.0099(11)	0.0006(10)
C6	0.0432(13)	0.0362(13)	0.0544(14)	-0.0080(11)	0.0106(11)	0.0084(10)
C7	0.0402(12)	0.0442(14)	0.0404(12)	-0.0035(10)	0.0142(10)	0.0078(10)
C7A	0.0303(11)	0.0363(12)	0.0349(11)	-0.0022(9)	0.0077(9)	0.0026(9)
C10	0.0424(14)	0.0491(15)	0.0583(16)	0.0066(12)	0.0089(12)	-0.0018(11)
C11	0.0540(15)	0.0365(13)	0.0398(12)	0.0017(10)	0.0105(11)	0.0074(11)
C12	0.0424(12)	0.0308(11)	0.0443(13)	0.0002(10)	0.0057(10)	0.0038(10)
C13	0.0571(16)	0.0394(14)	0.0427(13)	-0.0008(10)	0.0046(12)	0.0056(11)
C21	0.0343(12)	0.0398(13)	0.0458(13)	-0.0008(10)	0.0108(10)	-0.0050(10)
C22	0.0420(14)	0.0643(18)	0.0533(15)	-0.0129(13)	0.0039(12)	-0.0107(12)
C23	0.0371(13)	0.085(2)	0.0609(17)	-0.0125(15)	0.0193(12)	-0.0044(13)
C24	0.0504(13)	0.0256(11)	0.0305(10)	0.0031(8)	0.0078(9)	-0.0038(9)
C25	0.0629(16)	0.0415(13)	0.0316(11)	-0.0017(10)	0.0102(11)	-0.0035(11)
C26	0.0485(14)	0.0385(13)	0.0462(13)	0.0041(10)	-0.0025(11)	0.0076(11)
C27	0.101(2)	0.0390(14)	0.0335(12)	0.0059(10)	0.0144(13)	0.0119(14)
C28	0.0675(17)	0.0433(14)	0.0629(17)	-0.0115(12)	0.0395(14)	-0.0207(12)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table 8c. Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms for **5b**.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1A	0.3378	0.1715	-0.1788	0.046
H1B	0.4553	0.1788	-0.1117	0.046
H4	0.2397	-0.0158	0.0927	0.044
H5	0.2984	-0.1567	0.0329	0.050
H6	0.3909	-0.1582	-0.0986	0.053
H7	0.4324	-0.0188	-0.1703	0.049
H21	0.0714	0.0945	0.1152	0.047
H22A	0.0700	0.1113	-0.0452	0.064
H22B	-0.0025	0.2048	-0.0426	0.064
H22C	-0.0555	0.1071	-0.0174	0.064
H23A	0.0050	0.2148	0.2050	0.072
H23B	-0.0956	0.1708	0.1361	0.072
H23C	-0.0430	0.2692	0.1128	0.072
H24	0.2338	0.1069	0.2219	0.042
H25A	0.1558	0.2357	0.2934	0.054
H25B	0.2726	0.2904	0.2943	0.054
H25C	0.2668	0.1977	0.3544	0.054
H26A	0.4094	0.1212	0.1637	0.054
H26B	0.4236	0.1268	0.2741	0.054
H26C	0.4288	0.2198	0.2143	0.054
H27A	0.2402	0.4160	-0.1429	0.069
H27B	0.1715	0.3201	-0.1483	0.069
H27C	0.2893	0.3265	-0.1898	0.069
H28A	0.4215	0.4261	-0.0438	0.066
H28B	0.4609	0.3355	-0.0952	0.066
H28C	0.4684	0.3373	0.0151	0.066

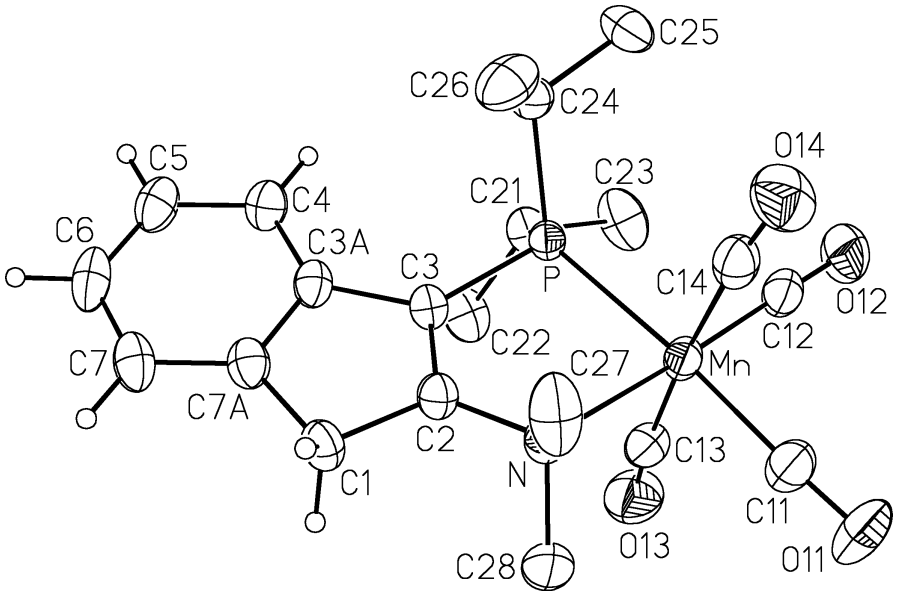

Figure 1d. Perspective view of the [{κ^2–(2-Me$_2$N-1*H*-inden-3-yl)P^{i}Pr$_2$}Mn(CO)$_4$]$^+$ complex ion showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 50% probability level. Hydrogen atoms are shown with arbitrarily small thermal parameters for the indenyl group, and are not shown for the methyl or isopropyl groups.

Table 1d. Crystallographic Experimental Details for **6**.

A. Crystal Data	
formula	$C_{21}H_{26}BF_4MnNO_4P$
formula weight	529.15
crystal dimensions (mm)	$0.46 \times 0.36 \times 0.26$
crystal system	monoclinic
space group	$P2_1/c$ (No. 14)
unit cell parameters[a]	
a (Å)	8.1358 (4)
b (Å)	19.1164 (9)
c (Å)	15.9808 (7)
β (deg)	96.3604 (9)
V (Å^3)	2470.2 (2)
Z	4
ρ_{calcd} (g cm^{-3})	1.423
μ (mm^{-1})	0.656
B. Data Collection and Refinement Conditions	
diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.2°) (15 s exposures)
data collection 2θ limit (deg)	52.78
total data collected	18344 ($-10 \le h \le 10$, $-23 \le k \le 23$, $-19 \le l \le 19$)
independent reflections	5048 (R_{int} = 0.0240)
number of observed reflections (*NO*)	4530 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–86*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	multi-scan (*SADABS*)
range of transmission factors	0.8480–0.7524
data/restraints/parameters	5048 [$F_o^2 \ge -3\sigma(F_o^2)$] / 0 / 296
goodness-of-fit (S)[e]	1.043 [$F_o^2 \ge -3\sigma(F_o^2)$]
final R indices[f]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0479
wR_2 [$F_o^2 \ge -3\sigma(F_o^2)$]	0.1295
largest difference peak and hole	1.453 and –0.679 e Å^{-3}

[a]Obtained from least-squares refinement of 6027 reflections with $4.98° < 2\theta < 52.74°$.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table 1d. Crystallographic Experimental Details for **6**. (continued)

[c]Sheldrick, G. M. *Acta Crystallogr.* **1990**, *A46*, 467–473.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted *R*-factors wR_2 and all goodnesses of fit *S* are based on F_o^2; conventional *R*-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. *R*-factors based on F_o^2 are statistically about twice as large as those based on F_o, and *R*-factors based on ALL data will be even larger.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0662P)^2 + 3.0015P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2d. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for **6**.

(a) atoms of [{ κ²–(2-Me₂N-1H-inden-3-yl)P^{i}Pr₂}Mn(CO)₄]⁺

Atom	*x*	*y*	*z*	U_{eq}, Å²
Mn	0.07578(5)	0.459099(18)	0.19175(2)	0.02872(13)*
P	0.16057(7)	0.34261(3)	0.20501(4)	0.02426(15)*
O11	-0.0075(3)	0.61019(11)	0.16931(16)	0.0599(6)*
O12	-0.1179(3)	0.43603(12)	0.02706(13)	0.0538(6)*
O13	0.3730(3)	0.49413(13)	0.10567(16)	0.0592(6)*
O14	-0.2546(3)	0.43569(13)	0.25445(16)	0.0558(6)*
N	0.2208(3)	0.47215(11)	0.31504(14)	0.0349(5)*
C1	0.4572(3)	0.40800(14)	0.41131(15)	0.0336(5)*
C2	0.3264(3)	0.41160(13)	0.33677(15)	0.0288(5)*
C3	0.3099(3)	0.35045(13)	0.29551(14)	0.0272(5)*
C3A	0.4236(3)	0.29878(13)	0.33951(15)	0.0296(5)*
C4	0.4499(3)	0.22847(14)	0.32375(17)	0.0364(6)*
C5	0.5674(3)	0.19277(15)	0.37740(18)	0.0406(6)*
C6	0.6560(3)	0.22636(16)	0.44438(18)	0.0430(7)*
C7	0.6302(3)	0.29680(16)	0.46038(16)	0.0391(6)*
C7A	0.5122(3)	0.33278(14)	0.40781(15)	0.0318(5)*
C11	0.0241(4)	0.55349(15)	0.18262(18)	0.0408(6)*
C12	-0.0402(3)	0.44417(14)	0.09050(17)	0.0367(6)*
C13	0.2642(4)	0.47845(14)	0.14000(18)	0.0389(6)*
C14	-0.1250(3)	0.44317(14)	0.23649(17)	0.0372(6)*
C21	0.2695(3)	0.30178(14)	0.12133(16)	0.0331(5)*
C22	0.4535(3)	0.32017(17)	0.12809(18)	0.0437(7)*
C23	0.1883(4)	0.3162(2)	0.03204(18)	0.0520(8)*
C24	0.0227(3)	0.27228(13)	0.23453(17)	0.0328(5)*
C25	-0.1194(4)	0.25863(17)	0.1659(2)	0.0499(7)*
C26	-0.0376(4)	0.28459(17)	0.3203(2)	0.0495(7)*
C27	0.1088(4)	0.4802(2)	0.38317(18)	0.0535(8)*
C28	0.3285(5)	0.53616(15)	0.3186(2)	0.0562(9)*

(b) tetrafluoroborate ion atoms

Atom	*x*	*y*	*z*	U_{eq}, Å²
F1	-0.2678(2)	0.53649(8)	0.41183(11)	0.0490(4)*
F2	-0.3948(2)	0.64024(10)	0.38252(15)	0.0649(6)*
F3A[a]	-0.1813(5)	0.6069(2)	0.3125(3)	0.0766(10)
F4A[a]	-0.1344(5)	0.6371(2)	0.4451(3)	0.0800(11)
F3B[b]	-0.2827(8)	0.5842(3)	0.2833(4)	0.0736(15)
F4B[b]	-0.1147(8)	0.6304(3)	0.3807(4)	0.0778(16)

Table 2d. Atomic Coordinates and Displacement Parameters for **6**. (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
B1A[a]	-0.2419(7)	0.6051(3)	0.3895(4)	0.0349(13)
B1B[b]	-0.2742(12)	0.5979(5)	0.3641(7)	0.038(2)

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$. [a]Refined with an occupancy factor of 0.6. [b]Refined with an occupancy factor of 0.4.

Table 3d. Selected Interatomic Distances (Å) for **6**.

(a) within [{κ²–(2-Me₂N-1H-inden-3-yl)P^{i}Pr₂}Mn(CO)₄]⁺

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Mn	P	2.3340(7)	N	C28	1.502(4)
Mn	N	2.196(2)	C1	C2	1.509(3)
Mn	C11	1.855(3)	C1	C7A	1.509(4)
Mn	C12	1.803(3)	C2	C3	1.341(3)
Mn	C13	1.858(3)	C3	C3A	1.477(3)
Mn	C14	1.879(3)	C3A	C4	1.388(4)
P	C3	1.789(2)	C3A	C7A	1.400(4)
P	C21	1.856(2)	C4	C5	1.391(4)
P	C24	1.845(2)	C5	C6	1.381(4)
O11	C11	1.129(3)	C6	C7	1.391(4)
O12	C12	1.144(3)	C7	C7A	1.386(3)
O13	C13	1.132(4)	C21	C22	1.530(4)
O14	C14	1.132(4)	C21	C23	1.530(4)
N	C2	1.460(3)	C24	C25	1.526(4)
N	C27	1.503(4)	C24	C26	1.524(4)

(b) within the tetrafluoroborate ion

Atom1	Atom2	Distance	Atom1	Atom2	Distance
F1	B1A	1.381(6)	F3A	B1A	1.376(7)
F1	B1B	1.398(9)	F4A	B1A	1.326(8)
F2	B1A	1.407(6)	F3B	B1B	1.311(12)
F2	B1B	1.331(9)	F4B	B1B	1.437(12)

Table 4d. Selected Interatomic Angles (deg) for **6**.

(a) within [{κ²–(2-Me₂N-1H-inden-3-yl)P^{i}Pr₂}Mn(CO)₄]⁺

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
P	Mn	N	84.43(6)	C2	C1	C7A	101.6(2)
P	Mn	C11	175.92(10)	N	C2	C1	124.7(2)
P	Mn	C12	92.90(9)	N	C2	C3	123.4(2)
P	Mn	C13	88.87(9)	C1	C2	C3	111.8(2)
P	Mn	C14	94.10(8)	P	C3	C2	119.50(18)
N	Mn	C11	93.13(11)	P	C3	C3A	131.46(19)
N	Mn	C12	177.32(10)	C2	C3	C3A	109.0(2)
N	Mn	C13	89.35(11)	C3	C3A	C4	131.5(2)
N	Mn	C14	94.62(10)	C3	C3A	C7A	107.6(2)
C11	Mn	C12	89.53(12)	C4	C3A	C7A	120.9(2)
C11	Mn	C13	87.84(13)	C3A	C4	C5	118.2(3)
C11	Mn	C14	89.34(13)	C4	C5	C6	120.9(3)
C12	Mn	C13	90.45(12)	C5	C6	C7	121.1(2)
C12	Mn	C14	85.70(12)	C6	C7	C7A	118.5(3)
C13	Mn	C14	175.25(12)	C1	C7A	C3A	110.0(2)
Mn	P	C3	99.25(8)	C1	C7A	C7	129.7(2)
Mn	P	C21	119.71(9)	C3A	C7A	C7	120.3(2)
Mn	P	C24	122.44(8)	Mn	C11	O11	173.7(3)
C3	P	C21	106.38(11)	Mn	C12	O12	177.8(3)
C3	P	C24	103.42(12)	Mn	C13	O13	175.1(3)
C21	P	C24	103.30(12)	Mn	C14	O14	172.0(3)
Mn	N	C2	111.52(15)	P	C21	C22	113.21(18)
Mn	N	C27	110.66(17)	P	C21	C23	113.88(19)
Mn	N	C28	112.30(18)	C22	C21	C23	110.0(2)
C2	N	C27	107.3(2)	P	C24	C25	112.00(19)
C2	N	C28	108.2(2)	P	C24	C26	112.50(19)
C27	N	C28	106.7(3)	C25	C24	C26	112.3(2)

(b) within the tetrafluoroborate ion

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
F1	B1A	F2	108.4(4)	F1	B1B	F2	112.0(6)
F1	B1A	F3A	109.6(5)	F1	B1B	F3B	111.4(7)
F1	B1A	F4A	111.9(5)	F1	B1B	F4B	106.5(7)
F2	B1A	F3A	108.6(5)	F2	B1B	F3B	112.3(8)
F2	B1A	F4A	110.1(5)	F2	B1B	F4B	111.6(7)
F3A	B1A	F4A	108.2(5)	F3B	B1B	F4B	102.5(7)

Table 5d. Torsional Angles (deg) for **6**.

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
N	Mn	P	C3	-9.60(10)	P	Mn	C13	O13	154(3)
N	Mn	P	C21	-124.56(11)	N	Mn	C13	O13	-121(3)
N	Mn	P	C24	102.87(12)	C11	Mn	C13	O13	-28(3)
C11	Mn	P	C3	43.7(13)	C12	Mn	C13	O13	61(3)
C11	Mn	P	C21	-71.3(13)	C14	Mn	C13	O13	25(4)
C11	Mn	P	C24	156.1(13)	P	Mn	C14	O14	-115.5(18)
C12	Mn	P	C3	170.26(12)	N	Mn	C14	O14	159.7(18)
C12	Mn	P	C21	55.30(13)	C11	Mn	C14	O14	66.6(18)
C12	Mn	P	C24	-77.28(14)	C12	Mn	C14	O14	-22.9(18)
C13	Mn	P	C3	79.86(12)	C13	Mn	C14	O14	13(3)
C13	Mn	P	C21	-35.10(13)	Mn	P	C3	C2	6.5(2)
C13	Mn	P	C24	-167.67(13)	Mn	P	C3	C3A	-176.2(2)
C14	Mn	P	C3	-103.85(11)	C21	P	C3	C2	131.4(2)
C14	Mn	P	C21	141.19(12)	C21	P	C3	C3A	-51.4(3)
C14	Mn	P	C24	8.62(13)	C24	P	C3	C2	-120.2(2)
P	Mn	N	C2	12.90(16)	C24	P	C3	C3A	57.1(2)
P	Mn	N	C27	-106.41(19)	Mn	P	C21	C22	80.6(2)
P	Mn	N	C28	134.5(2)	Mn	P	C21	C23	-46.1(2)
C11	Mn	N	C2	-163.83(19)	C3	P	C21	C22	-30.6(2)
C11	Mn	N	C27	76.9(2)	C3	P	C21	C23	-157.3(2)
C11	Mn	N	C28	-42.2(2)	C24	P	C21	C22	-139.1(2)
C12	Mn	N	C2	10(2)	C24	P	C21	C23	94.2(2)
C12	Mn	N	C27	-109(2)	Mn	P	C24	C25	67.8(2)
C12	Mn	N	C28	131(2)	Mn	P	C24	C26	-59.8(2)
C13	Mn	N	C2	-76.02(18)	C3	P	C24	C25	178.11(19)
C13	Mn	N	C27	164.7(2)	C3	P	C24	C26	50.5(2)
C13	Mn	N	C28	45.6(2)	C21	P	C24	C25	-71.1(2)
C14	Mn	N	C2	106.58(18)	C21	P	C24	C26	161.3(2)
C14	Mn	N	C27	-12.7(2)	Mn	N	C2	C1	171.52(19)
C14	Mn	N	C28	-131.8(2)	Mn	N	C2	C3	-13.3(3)
P	Mn	C11	O11	96(3)	C27	N	C2	C1	-67.2(3)
N	Mn	C11	O11	149(3)	C27	N	C2	C3	108.0(3)
C12	Mn	C11	O11	-31(3)	C28	N	C2	C1	47.6(3)
C13	Mn	C11	O11	60(3)	C28	N	C2	C3	-137.3(3)
C14	Mn	C11	O11	-117(3)	C7A	C1	C2	N	174.3(2)
P	Mn	C12	O12	138(7)	C7A	C1	C2	C3	-1.4(3)
N	Mn	C12	O12	141(6)	C2	C1	C7A	C3A	0.3(3)
C11	Mn	C12	O12	-45(7)	C2	C1	C7A	C7	-179.5(3)
C13	Mn	C12	O12	-133(7)	N	C2	C3	P	4.0(3)
C14	Mn	C12	O12	44(7)	N	C2	C3	C3A	-173.8(2)

Table 5d. Torsional Angles for **6**. (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C1	C2	C3	P	179.71(17)	C3	C3A	C7A	C7	-179.4(2)
C1	C2	C3	C3A	1.9(3)	C4	C3A	C7A	C1	-178.8(2)
P	C3	C3A	C4	0.4(4)	C4	C3A	C7A	C7	0.9(4)
P	C3	C3A	C7A	-179.13(19)	C3A	C4	C5	C6	-0.2(4)
C2	C3	C3A	C4	177.9(3)	C4	C5	C6	C7	0.1(4)
C2	C3	C3A	C7A	-1.7(3)	C5	C6	C7	C7A	0.4(4)
C3	C3A	C4	C5	-179.9(3)	C6	C7	C7A	C1	178.8(3)
C7A	C3A	C4	C5	-0.3(4)	C6	C7	C7A	C3A	-1.0(4)
C3	C3A	C7A	C1	0.8(3)					

Table 6d. Least-Squares Planes for **6**.

Plane	Coefficients[a]			Defining Atoms with Deviations (Å)[b]			
1	6.273(4)	4.908(12)	-10.621(10)	0.509(8)			
				C1	-0.007(2)	C2	-0.0180(19)
				C3	0.0166(19)	C3A	0.009(2)
				C4	-0.004(2)	C5	-0.012(2)
				C6	-0.003(2)	C7	0.011(2)
				C7A	0.006(2)		
				Mn	0.184(3)	P	0.003(3)
				N	-0.152(3)		

[a]Coefficients are for the form $ax+by+cz = d$ where x, y and z are crystallographic coordinates.
[b]Underlined atoms were not included in the definition of the plane.

Table 7d. Anisotropic Displacement Parameters (U_{ij}, Å^2) for **6**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mn	0.0329(2)	0.0243(2)	0.0278(2)	0.00153(13)	-0.00179(15)	0.00337(14)
P	0.0241(3)	0.0241(3)	0.0241(3)	-0.0006(2)	0.0007(2)	0.0019(2)
O11	0.0857(17)	0.0304(11)	0.0636(15)	0.0079(10)	0.0085(13)	0.0152(11)
O12	0.0602(13)	0.0574(13)	0.0391(11)	0.0030(10)	-0.0157(10)	0.0020(11)
O13	0.0530(13)	0.0574(14)	0.0695(16)	0.0127(12)	0.0173(12)	-0.0075(11)
O14	0.0404(12)	0.0616(14)	0.0672(15)	-0.0075(12)	0.0134(10)	0.0052(10)
N	0.0426(12)	0.0281(10)	0.0323(11)	-0.0055(8)	-0.0040(9)	0.0058(9)
C1	0.0346(12)	0.0381(14)	0.0265(12)	-0.0024(10)	-0.0028(10)	0.0019(11)
C2	0.0299(11)	0.0309(12)	0.0251(11)	0.0013(9)	0.0007(9)	0.0017(9)
C3	0.0260(11)	0.0306(12)	0.0246(11)	0.0005(9)	0.0006(9)	0.0030(9)
C3A	0.0283(11)	0.0347(13)	0.0258(11)	0.0050(9)	0.0037(9)	0.0042(10)
C4	0.0362(13)	0.0354(14)	0.0372(14)	0.0026(11)	0.0023(11)	0.0075(11)
C5	0.0401(14)	0.0392(14)	0.0434(15)	0.0087(12)	0.0086(12)	0.0133(12)
C6	0.0371(14)	0.0563(17)	0.0363(14)	0.0173(13)	0.0069(11)	0.0181(13)
C7	0.0351(13)	0.0552(17)	0.0266(12)	0.0060(11)	0.0011(10)	0.0066(12)
C7A	0.0296(12)	0.0400(14)	0.0261(12)	0.0034(10)	0.0044(9)	0.0029(10)
C11	0.0512(16)	0.0320(14)	0.0383(15)	0.0010(11)	0.0003(12)	0.0036(12)
C12	0.0412(14)	0.0313(12)	0.0360(14)	0.0047(10)	-0.0027(11)	0.0039(11)
C13	0.0441(15)	0.0309(13)	0.0407(15)	0.0045(11)	-0.0003(12)	-0.0007(11)
C14	0.0403(15)	0.0326(13)	0.0379(14)	-0.0019(11)	0.0002(11)	0.0070(11)
C21	0.0329(12)	0.0367(13)	0.0297(12)	-0.0059(10)	0.0037(10)	0.0049(10)
C22	0.0338(14)	0.0594(18)	0.0392(15)	-0.0039(13)	0.0102(11)	0.0071(13)
C23	0.0487(17)	0.077(2)	0.0295(14)	-0.0138(14)	0.0004(12)	0.0077(16)
C24	0.0271(11)	0.0275(12)	0.0439(14)	0.0041(10)	0.0046(10)	0.0012(9)
C25	0.0312(14)	0.0486(17)	0.068(2)	-0.0018(15)	-0.0039(13)	-0.0084(12)
C26	0.0519(17)	0.0431(16)	0.0574(19)	0.0118(14)	0.0237(15)	0.0014(13)
C27	0.0577(19)	0.067(2)	0.0342(15)	-0.0119(14)	-0.0009(13)	0.0302(16)
C28	0.070(2)	0.0302(15)	0.061(2)	-0.0043(13)	-0.0265(17)	-0.0039(14)
F1	0.0618(11)	0.0343(9)	0.0512(10)	0.0077(7)	0.0069(8)	-0.0026(7)
F2	0.0550(11)	0.0408(10)	0.1017(17)	0.0015(10)	0.0207(11)	0.0057(8)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table 8d. Derived Atomic Coordinates and Displacement Parameters for H-Atoms for **6**.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1A	0.4106	0.4183	0.4646	0.040
H1B	0.5494	0.4407	0.4049	0.040
H4	0.3892	0.2054	0.2776	0.044
H5	0.5871	0.1446	0.3678	0.049
H6	0.7358	0.2009	0.4801	0.052
H7	0.6920	0.3197	0.5063	0.047
H21	0.2632	0.2501	0.1298	0.040
H22A	0.5046	0.3106	0.1854	0.052
H22B	0.4662	0.3699	0.1153	0.052
H22C	0.5075	0.2918	0.0880	0.052
H23A	0.0712	0.3032	0.0279	0.062
H23B	0.2437	0.2887	-0.0083	0.062
H23C	0.1980	0.3661	0.0193	0.062
H24	0.0906	0.2286	0.2397	0.039
H25A	-0.0751	0.2511	0.1120	0.060
H25B	-0.1940	0.2990	0.1612	0.060
H25C	-0.1805	0.2169	0.1803	0.060
H26A	0.0576	0.2926	0.3624	0.059
H26B	-0.0989	0.2434	0.3362	0.059
H26C	-0.1102	0.3256	0.3174	0.059
H27A	0.0345	0.5200	0.3700	0.064
H27B	0.1755	0.4884	0.4372	0.064
H27C	0.0434	0.4375	0.3867	0.064
H28A	0.2603	0.5773	0.3028	0.067
H28B	0.4121	0.5308	0.2794	0.067
H28C	0.3834	0.5421	0.3759	0.067

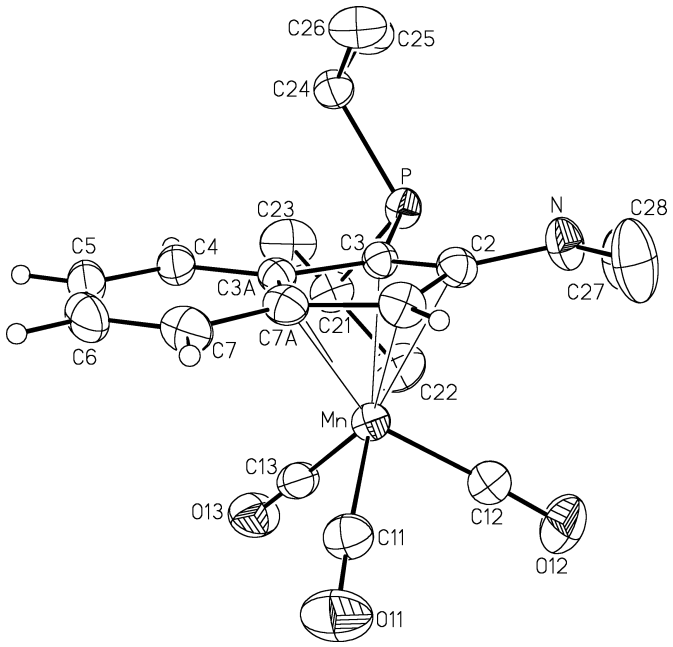

Figure 1e. Perspective view of the 2-dimethylamino-3-diisopropylphosphino-η^5-indenyl-tricarbonylmanganese molecule showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 50% probability level. Hydrogen atoms are shown with arbitrarily small thermal parameters for the indenyl group, and are not shown for the diisopropylphosphine and dimethylamine groups.

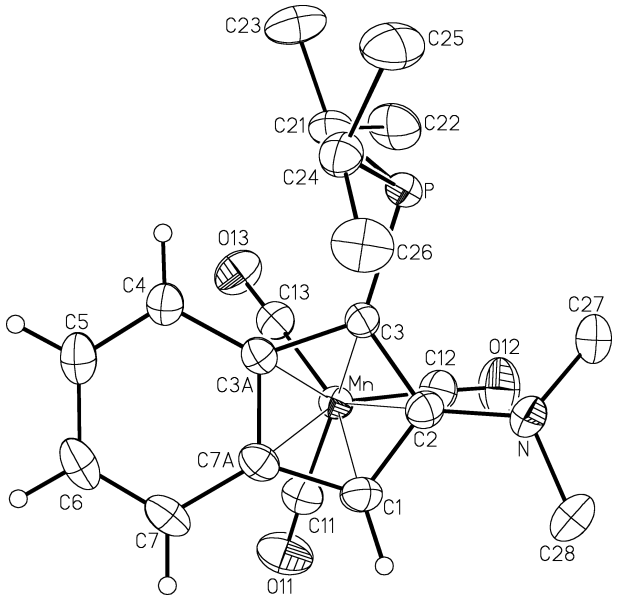

Figure 2e. Alternative view of of η^5-[**2**]Mn(CO)$_3$.

Table 1e. Crystallographic Experimental Details for η^5-[**2**]$Mn(CO)_3$.

A. Crystal Data	
formula	$C_{20}H_{25}MnNO_3P$
formula weight	413.32
crystal dimensions (mm)	$0.35 \times 0.30 \times 0.12$
crystal system	monoclinic
space group	$P2_1/n$ (an alternate setting of $P2_1/c$ [No. 14])
unit cell parameters[a]	
a (Å)	9.0105 (5)
b (Å)	24.9564 (14)
c (Å)	9.4436 (5)
β (deg)	108.4350 (10)
V (Å^3)	2014.60 (19)
Z	4
ρ_{calcd} (g cm^{-3})	1.363
μ (mm^{-1})	0.753
B. Data Collection and Refinement Conditions	
diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.2°) (20 s exposures)
data collection 2θ limit (deg)	52.78
total data collected	13161 ($-11 \le h \le 11$, $-31 \le k \le 31$, $-9 \le l \le 11$)
independent reflections	4123 (R_{int} = 0.0228)
number of observed reflections (*NO*)	3725 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–86*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	multi-scan (*SADABS*)
range of transmission factors	0.9151–0.7785
data/restraints/parameters	4123 [$F_o^2 \ge -3\sigma(F_o^2)$] / 0 / 237
goodness-of-fit (S)[e]	1.048 [$F_o^2 \ge -3\sigma(F_o^2)$]
final R indices[f]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0317
wR_2 [$F_o^2 \ge -3\sigma(F_o^2)$]	0.0873
largest difference peak and hole	0.416 and –0.313 e Å^{-3}

[a]Obtained from least-squares refinement of 4783 reflections with $5.04° < 2\theta < 52.72°$.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table 1e. Crystallographic Experimental Details for η^5-[**2**]$Mn(CO)_3$. (continued)

[c]Sheldrick, G. M. *Acta Crystallogr*. **1990**, *A46*, 467–473.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted *R*-factors wR_2 and all goodnesses of fit *S* are based on F_o^2; conventional *R*-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. *R*-factors based on F_o^2 are statistically about twice as large as those based on F_o, and *R*-factors based on ALL data will be even larger.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0515P)^2 + 0.6942P]^{-1}$ where $P = [\text{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2e. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for η^5-[**2**]$Mn(CO)_3$.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Mn	0.15170(3)	0.124406(9)	0.44588(3)	0.02399(9)*
P	0.27834(5)	0.165274(17)	0.12531(5)	0.02657(11)*
O11	0.0579(2)	0.08989(6)	0.70284(18)	0.0549(4)*
O12	-0.15952(17)	0.17297(7)	0.32459(19)	0.0581(4)*
O13	0.29343(16)	0.22481(6)	0.59361(17)	0.0444(3)*
N	-0.00606(17)	0.07257(6)	0.10991(17)	0.0346(3)*
C1	0.15329(19)	0.04483(6)	0.36332(19)	0.0292(3)*
C2	0.12256(18)	0.07857(6)	0.23514(18)	0.0266(3)*
C3	0.24817(17)	0.11763(6)	0.26196(18)	0.0230(3)*
C3A	0.36599(18)	0.10072(6)	0.39941(17)	0.0237(3)*
C4	0.52250(19)	0.11871(6)	0.47274(19)	0.0286(3)*
C5	0.6085(2)	0.09405(7)	0.6008(2)	0.0358(4)*
C6	0.5460(2)	0.05171(7)	0.6652(2)	0.0383(4)*
C7	0.3984(2)	0.03294(7)	0.5987(2)	0.0340(4)*
C7A	0.30678(19)	0.05655(6)	0.46182(18)	0.0273(3)*
C11	0.0975(2)	0.10383(7)	0.6043(2)	0.0345(4)*
C12	-0.0371(2)	0.15447(7)	0.3689(2)	0.0349(4)*
C13	0.23774(19)	0.18626(7)	0.53525(19)	0.0301(4)*
C21	0.3509(2)	0.22574(7)	0.2449(2)	0.0327(4)*
C22	0.2086(3)	0.26106(8)	0.2322(3)	0.0495(5)*
C23	0.4755(3)	0.25736(8)	0.2026(3)	0.0518(5)*
C24	0.4510(2)	0.13463(7)	0.0865(2)	0.0323(4)*
C25	0.4686(3)	0.16129(9)	-0.0538(3)	0.0499(5)*
C26	0.4235(3)	0.07472(8)	0.0582(3)	0.0447(5)*
C27	-0.0782(2)	0.11785(9)	0.0166(2)	0.0464(5)*
C28	-0.1158(3)	0.03050(10)	0.1146(3)	0.0617(7)*

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$.

Table 3e. Selected Interatomic Distances (Å) for η^5-[**2**]Mn(CO)$_3$.

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Mn	C1	2.1353(16)	N	C28	1.452(2)
Mn	C2	2.2378(16)	C1	C2	1.428(2)
Mn	C3	2.1808(16)	C1	C7A	1.432(2)
Mn	C3A	2.1924(15)	C2	C3	1.454(2)
Mn	C7A	2.1703(16)	C3	C3A	1.456(2)
Mn	C11	1.7893(18)	C3A	C4	1.433(2)
Mn	C12	1.7900(18)	C3A	C7A	1.430(2)
Mn	C13	1.8117(18)	C4	C5	1.360(2)
P	C3	1.8370(16)	C5	C6	1.421(3)
P	C21	1.8744(18)	C6	C7	1.361(3)
P	C24	1.8708(18)	C7	C7A	1.423(2)
O11	C11	1.151(2)	C21	C22	1.529(3)
O12	C12	1.146(2)	C21	C23	1.526(3)
O13	C13	1.143(2)	C24	C25	1.535(3)
N	C2	1.377(2)	C24	C26	1.525(3)
N	C27	1.454(2)			

Table 4e. Selected Interatomic Angles (deg) for η^5-[**2**]$Mn(CO)_3$.

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C1	Mn	C2	38.03(6)	Mn	C2	N	130.49(12)
C1	Mn	C3	65.59(6)	Mn	C2	C1	67.09(9)
C1	Mn	C3A	64.41(6)	Mn	C2	C3	68.68(9)
C1	Mn	C7A	38.83(6)	N	C2	C1	123.28(14)
C1	Mn	C11	94.21(7)	N	C2	C3	128.29(15)
C1	Mn	C12	110.91(7)	C1	C2	C3	108.43(14)
C1	Mn	C13	155.68(7)	Mn	C3	P	133.96(8)
C2	Mn	C3	38.40(6)	Mn	C3	C2	72.92(9)
C2	Mn	C3A	63.08(6)	Mn	C3	C3A	70.99(9)
C2	Mn	C7A	63.56(6)	P	C3	C2	126.27(12)
C2	Mn	C11	127.62(7)	P	C3	C3A	125.87(11)
C2	Mn	C12	91.37(7)	C2	C3	C3A	105.60(13)
C2	Mn	C13	139.68(7)	Mn	C3A	C3	70.13(8)
C3	Mn	C3A	38.88(6)	Mn	C3A	C4	127.83(11)
C3	Mn	C7A	65.46(6)	Mn	C3A	C7A	70.03(9)
C3	Mn	C11	157.89(7)	C3	C3A	C4	131.99(15)
C3	Mn	C12	106.03(7)	C3	C3A	C7A	109.21(13)
C3	Mn	C13	102.56(7)	C4	C3A	C7A	118.74(14)
C3A	Mn	C7A	38.27(6)	C3A	C4	C5	119.01(16)
C3A	Mn	C11	125.47(7)	C4	C5	C6	121.69(17)
C3A	Mn	C12	144.68(7)	C5	C6	C7	121.35(16)
C3A	Mn	C13	92.79(6)	C6	C7	C7A	118.54(17)
C7A	Mn	C11	93.32(7)	Mn	C7A	C1	69.26(9)
C7A	Mn	C12	149.74(7)	Mn	C7A	C3A	71.70(9)
C7A	Mn	C13	117.47(7)	Mn	C7A	C7	124.19(12)
C11	Mn	C12	89.10(8)	C1	C7A	C3A	107.41(14)
C11	Mn	C13	92.57(8)	C1	C7A	C7	132.02(16)
C12	Mn	C13	92.51(8)	C3A	C7A	C7	120.57(15)
C3	P	C21	101.45(8)	Mn	C11	O11	177.61(18)
C3	P	C24	100.94(7)	Mn	C12	O12	177.20(19)
C21	P	C24	107.10(8)	Mn	C13	O13	178.88(17)
C2	N	C27	121.95(15)	P	C21	C22	107.04(13)
C2	N	C28	116.63(16)	P	C21	C23	113.81(14)
C27	N	C28	113.74(16)	C22	C21	C23	110.45(16)
Mn	C1	C2	74.88(9)	P	C24	C25	108.12(13)
Mn	C1	C7A	71.91(9)	P	C24	C26	109.64(12)
C2	C1	C7A	108.59(14)	C25	C24	C26	109.18(16)

Table 5e. Torsional Angles (deg) for η^5-[**2**]Mn(CO)$_3$.

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C2	Mn	C1	C7A	115.83(13)	C7A	Mn	C3	C3A	-36.03(9)
C3	Mn	C1	C2	-35.24(9)	C11	Mn	C3	P	-175.33(16)
C3	Mn	C1	C7A	80.59(10)	C11	Mn	C3	C2	60.4(2)
C3A	Mn	C1	C2	-78.31(10)	C11	Mn	C3	C3A	-53.4(2)
C3A	Mn	C1	C7A	37.52(9)	C12	Mn	C3	P	53.10(13)
C7A	Mn	C1	C2	-115.83(13)	C12	Mn	C3	C2	-71.19(10)
C11	Mn	C1	C2	154.10(10)	C12	Mn	C3	C3A	175.02(10)
C11	Mn	C1	C7A	-90.07(11)	C13	Mn	C3	P	-43.26(12)
C12	Mn	C1	C2	63.46(11)	C13	Mn	C3	C2	-167.55(9)
C12	Mn	C1	C7A	179.29(10)	C13	Mn	C3	C3A	78.66(10)
C13	Mn	C1	C2	-100.12(18)	C1	Mn	C3A	C3	82.18(9)
C13	Mn	C1	C7A	15.7(2)	C1	Mn	C3A	C4	-149.50(16)
C1	Mn	C2	N	114.99(19)	C1	Mn	C3A	C7A	-38.06(9)
C1	Mn	C2	C3	-122.23(13)	C2	Mn	C3A	C3	39.60(8)
C3	Mn	C2	N	-122.78(19)	C2	Mn	C3A	C4	167.92(16)
C3	Mn	C2	C1	122.23(13)	C2	Mn	C3A	C7A	-80.64(10)
C3A	Mn	C2	N	-162.89(17)	C3	Mn	C3A	C4	128.32(18)
C3A	Mn	C2	C1	82.12(10)	C3	Mn	C3A	C7A	-120.24(13)
C3A	Mn	C2	C3	-40.10(9)	C7A	Mn	C3A	C3	120.24(13)
C7A	Mn	C2	N	154.07(17)	C7A	Mn	C3A	C4	-111.44(18)
C7A	Mn	C2	C1	39.08(9)	C11	Mn	C3A	C3	158.21(10)
C7A	Mn	C2	C3	-83.15(10)	C11	Mn	C3A	C4	-73.47(17)
C11	Mn	C2	N	81.63(17)	C11	Mn	C3A	C7A	37.97(13)
C11	Mn	C2	C1	-33.37(13)	C12	Mn	C3A	C3	-8.30(16)
C11	Mn	C2	C3	-155.59(10)	C12	Mn	C3A	C4	120.02(17)
C12	Mn	C2	N	-8.29(16)	C12	Mn	C3A	C7A	-128.55(13)
C12	Mn	C2	C1	-123.29(11)	C13	Mn	C3A	C3	-106.63(10)
C12	Mn	C2	C3	114.49(10)	C13	Mn	C3A	C4	21.69(15)
C13	Mn	C2	N	-103.80(16)	C13	Mn	C3A	C7A	133.13(10)
C13	Mn	C2	C1	141.21(12)	C1	Mn	C7A	C3A	117.54(13)
C13	Mn	C2	C3	18.98(14)	C1	Mn	C7A	C7	-127.45(19)
C1	Mn	C3	P	159.20(13)	C2	Mn	C7A	C1	-38.26(9)
C1	Mn	C3	C2	34.91(9)	C2	Mn	C7A	C3A	79.27(10)
C1	Mn	C3	C3A	-78.88(9)	C2	Mn	C7A	C7	-165.71(17)
C2	Mn	C3	P	124.29(15)	C3	Mn	C7A	C1	-80.94(10)
C2	Mn	C3	C3A	-113.79(12)	C3	Mn	C7A	C3A	36.59(9)
C3A	Mn	C3	P	-121.92(15)	C3	Mn	C7A	C7	151.61(17)
C3A	Mn	C3	C2	113.79(12)	C3A	Mn	C7A	C1	-117.54(13)
C7A	Mn	C3	P	-157.95(13)	C3A	Mn	C7A	C7	115.02(18)
C7A	Mn	C3	C2	77.76(9)	C11	Mn	C7A	C1	92.59(11)

Table 5e. Torsional Angles for η^5-[**2**]Mn(CO)$_3$. (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C11	Mn	C7A	C3A	-149.87(10)	C3	P	C24	C26	47.33(14)
C11	Mn	C7A	C7	-34.86(16)	C21	P	C24	C25	-88.00(14)
C12	Mn	C7A	C1	-1.32(19)	C21	P	C24	C26	153.06(13)
C12	Mn	C7A	C3A	116.22(16)	C27	N	C2	Mn	62.5(2)
C12	Mn	C7A	C7	-128.77(18)	C27	N	C2	C1	149.54(18)
C13	Mn	C7A	C1	-172.78(10)	C27	N	C2	C3	-31.2(3)
C13	Mn	C7A	C3A	-55.24(11)	C28	N	C2	Mn	-85.0(2)
C13	Mn	C7A	C7	59.77(17)	C28	N	C2	C1	2.0(3)
C1	Mn	C11	O11	-62(4)	C28	N	C2	C3	-178.73(19)
C2	Mn	C11	O11	-42(4)	Mn	C1	C2	N	-124.46(16)
C3	Mn	C11	O11	-85(4)	Mn	C1	C2	C3	56.16(11)
C3A	Mn	C11	O11	-123(4)	C7A	C1	C2	Mn	-64.51(11)
C7A	Mn	C11	O11	-101(4)	C7A	C1	C2	N	171.02(15)
C12	Mn	C11	O11	49(4)	C7A	C1	C2	C3	-8.35(18)
C13	Mn	C11	O11	141(4)	Mn	C1	C7A	C3A	-61.92(11)
C1	Mn	C12	O12	92(4)	Mn	C1	C7A	C7	117.88(19)
C2	Mn	C12	O12	126(4)	C2	C1	C7A	Mn	66.46(11)
C3	Mn	C12	O12	162(4)	C2	C1	C7A	C3A	4.54(18)
C3A	Mn	C12	O12	167(4)	C2	C1	C7A	C7	-175.66(17)
C7A	Mn	C12	O12	93(4)	Mn	C2	C3	P	-132.47(12)
C11	Mn	C12	O12	-2(4)	Mn	C2	C3	C3A	63.92(10)
C13	Mn	C12	O12	-94(4)	N	C2	C3	Mn	125.45(17)
C1	Mn	C13	O13	-54(8)	N	C2	C3	P	-7.0(2)
C2	Mn	C13	O13	-124(8)	N	C2	C3	C3A	-170.63(16)
C3	Mn	C13	O13	-112(8)	C1	C2	C3	Mn	-55.22(11)
C3A	Mn	C13	O13	-74(8)	C1	C2	C3	P	172.31(12)
C7A	Mn	C13	O13	-43(8)	C1	C2	C3	C3A	8.70(17)
C11	Mn	C13	O13	52(8)	Mn	C3	C3A	C4	-123.52(17)
C12	Mn	C13	O13	141(8)	Mn	C3	C3A	C7A	59.30(11)
C21	P	C3	Mn	41.38(12)	P	C3	C3A	Mn	131.06(12)
C21	P	C3	C2	143.00(14)	P	C3	C3A	C4	7.5(2)
C21	P	C3	C3A	-56.60(15)	P	C3	C3A	C7A	-169.64(11)
C24	P	C3	Mn	151.55(11)	C2	C3	C3A	Mn	-65.25(10)
C24	P	C3	C2	-106.83(14)	C2	C3	C3A	C4	171.23(16)
C24	P	C3	C3A	53.58(14)	C2	C3	C3A	C7A	-5.95(17)
C3	P	C21	C22	-93.89(14)	Mn	C3A	C4	C5	84.75(19)
C3	P	C21	C23	143.78(15)	C3	C3A	C4	C5	-178.36(16)
C24	P	C21	C22	160.74(13)	C7A	C3A	C4	C5	-1.4(2)
C24	P	C21	C23	38.42(17)	Mn	C3A	C7A	C1	60.35(11)
C3	P	C24	C25	166.27(13)	Mn	C3A	C7A	C7	-119.47(15)

Table 5e. Torsional Angles for η^5-[**2**]Mn(CO)$_3$. (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C3	C3A	C7A	Mn	-59.36(11)	C3A	C4	C5	C6	-1.3(3)
C3	C3A	C7A	C1	0.99(18)	C4	C5	C6	C7	2.0(3)
C3	C3A	C7A	C7	-178.84(14)	C5	C6	C7	C7A	0.2(3)
C4	C3A	C7A	Mn	123.03(14)	C6	C7	C7A	Mn	-90.68(19)
C4	C3A	C7A	C1	-176.62(14)	C6	C7	C7A	C1	177.27(17)
C4	C3A	C7A	C7	3.6(2)	C6	C7	C7A	C3A	-3.0(2)

Table 6e. Least-Squares Planes for η^5-[**2**]$Mn(CO)_3$.

Plane	Coefficients[a]			Defining Atoms with Deviations (Å)[b]			
1	-5.460(6)	15.750(16)	6.148(6)	2.065(3)			
				C1	0.0381(10)	C2	-0.0507(10)
				C3	0.0436(10)	C3A	-0.0212(10)
				C7A	-0.0098(10)		
				N	-0.213(3)	P	-0.211(3)
				Mn	1.8078(7)		
2	-4.920(5)	16.326(13)	6.319(5)	2.352(4)			
				C3A	0.0151(11)	C4	0.0022(12)
				C5	-0.0142(13)	C6	0.0088(13)
				C7	0.0085(12)	C7A	-0.0204(11)

Dihedral angle between planes 1 and 2: 4.31(12)°

[a]Coefficients are for the form $ax+by+cz = d$ where x, y and z are crystallographic coordinates.
[b]Underlined atoms were not included in the definition of the plane.

Table 7e. Anisotropic Displacement Parameters (U_{ij}, Å^2) for η^5-[**2**]Mn(CO)$_3$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mn	0.02459(14)	0.02339(14)	0.02455(15)	0.00111(9)	0.00856(10)	0.00078(8)
P	0.0258(2)	0.0275(2)	0.0257(2)	0.00591(16)	0.00719(17)	-0.00034(15)
O11	0.0714(10)	0.0570(9)	0.0486(9)	0.0112(7)	0.0366(8)	0.0010(8)
O12	0.0343(8)	0.0696(10)	0.0625(11)	-0.0006(8)	0.0043(7)	0.0168(7)
O13	0.0471(8)	0.0396(7)	0.0492(8)	-0.0154(6)	0.0190(7)	-0.0081(6)
N	0.0313(7)	0.0371(8)	0.0302(8)	-0.0010(6)	0.0024(6)	-0.0103(6)
C1	0.0340(8)	0.0232(7)	0.0313(9)	0.0003(6)	0.0117(7)	-0.0034(6)
C2	0.0280(8)	0.0249(7)	0.0268(8)	-0.0025(6)	0.0086(6)	-0.0016(6)
C3	0.0232(7)	0.0227(7)	0.0226(8)	0.0003(6)	0.0065(6)	0.0002(6)
C3A	0.0269(7)	0.0213(7)	0.0224(8)	-0.0008(6)	0.0071(6)	0.0026(6)
C4	0.0271(8)	0.0277(8)	0.0288(9)	-0.0028(6)	0.0059(7)	0.0020(6)
C5	0.0311(8)	0.0382(9)	0.0314(9)	-0.0061(7)	0.0002(7)	0.0056(7)
C6	0.0460(10)	0.0374(9)	0.0250(9)	0.0028(7)	0.0020(7)	0.0145(8)
C7	0.0477(10)	0.0261(8)	0.0283(9)	0.0062(7)	0.0123(8)	0.0094(7)
C7A	0.0343(8)	0.0218(7)	0.0263(8)	0.0006(6)	0.0103(7)	0.0040(6)
C11	0.0373(9)	0.0329(9)	0.0357(10)	0.0023(7)	0.0147(8)	0.0024(7)
C12	0.0322(9)	0.0378(9)	0.0345(10)	-0.0028(7)	0.0102(7)	0.0007(7)
C13	0.0292(8)	0.0328(9)	0.0312(9)	-0.0002(7)	0.0136(7)	0.0034(7)
C21	0.0373(9)	0.0235(8)	0.0394(10)	0.0028(7)	0.0152(8)	-0.0008(7)
C22	0.0559(12)	0.0308(10)	0.0638(14)	0.0077(9)	0.0217(11)	0.0133(9)
C23	0.0622(13)	0.0355(10)	0.0666(15)	-0.0032(10)	0.0332(12)	-0.0169(9)
C24	0.0298(8)	0.0385(9)	0.0301(9)	-0.0018(7)	0.0116(7)	-0.0019(7)
C25	0.0605(13)	0.0551(12)	0.0452(12)	-0.0009(10)	0.0325(11)	-0.0095(10)
C26	0.0543(12)	0.0390(10)	0.0484(12)	-0.0032(9)	0.0269(10)	0.0048(9)
C27	0.0336(10)	0.0557(12)	0.0386(11)	0.0072(9)	-0.0048(8)	-0.0066(8)
C28	0.0511(12)	0.0585(14)	0.0589(15)	0.0053(11)	-0.0064(11)	-0.0305(11)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table 8e. Derived Atomic Coordinates and Displacement Parameters for H-Atoms for η^5-[**2**]Mn(CO)$_3$.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1	0.0851	0.0147	0.3757	0.035
H4	0.5656	0.1474	0.4325	0.034
H5	0.7131	0.1054	0.6485	0.043
H6	0.6084	0.0362	0.7564	0.046
H7	0.3575	0.0047	0.6428	0.041
H21	0.3960	0.2138	0.3510	0.039
H22A	0.2420	0.2933	0.2932	0.059
H22B	0.1335	0.2411	0.2676	0.059
H22C	0.1592	0.2714	0.1277	0.059
H23A	0.5063	0.2887	0.2679	0.062
H23B	0.4332	0.2692	0.0986	0.062
H23C	0.5670	0.2345	0.2141	0.062
H24	0.5476	0.1406	0.1732	0.039
H25A	0.5592	0.1460	-0.0756	0.060
H25B	0.4838	0.1999	-0.0369	0.060
H25C	0.3739	0.1549	-0.1385	0.060
H26A	0.5150	0.0586	0.0399	0.054
H26B	0.3309	0.0692	-0.0293	0.054
H26C	0.4068	0.0578	0.1456	0.054
H27A	-0.0053	0.1324	-0.0317	0.056
H27B	-0.1037	0.1457	0.0785	0.056
H27C	-0.1741	0.1060	-0.0598	0.056
H28A	-0.0587	-0.0030	0.1475	0.074
H28B	-0.1913	0.0256	0.0149	0.074
H28C	-0.1713	0.0405	0.1847	0.074

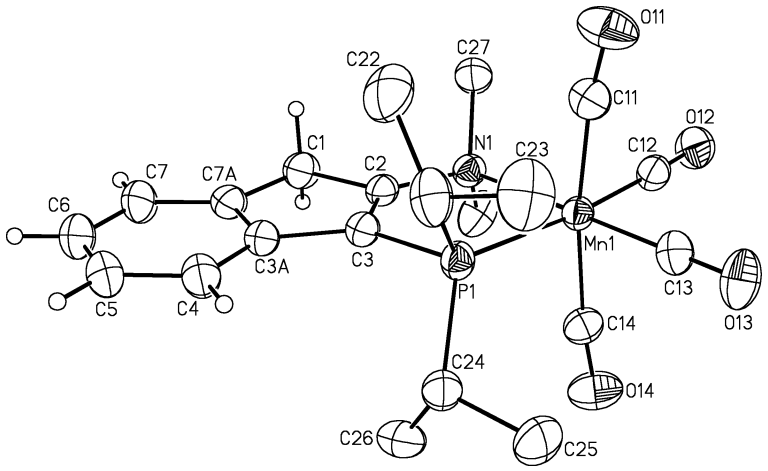

Figure 1f. Perspective view of the [{κ^2–(2-Me$_2$N-1*H*-inden-3-yl)P^{i}Pr$_2$}Mn(CO)$_4$]$^+$ cation showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 50% probability level. Hydrogen atoms are shown with arbitrarily small thermal parameters for the indenyl group; all other hydrogens are not shown.

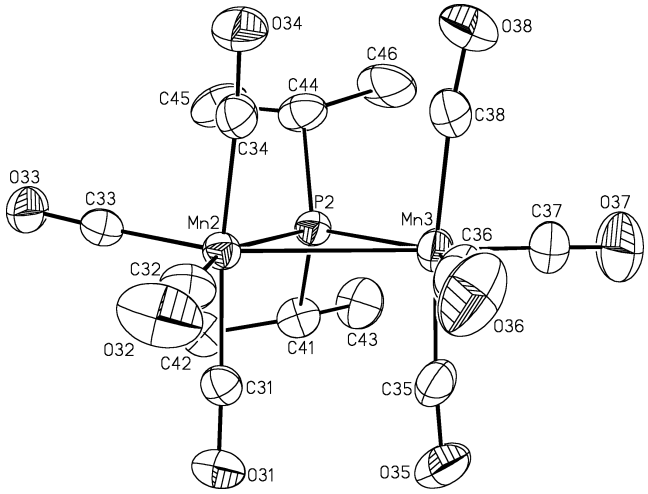

Figure 2f. Perspective view of the [Mn$_2$(CO)$_8$(μ–P^{i}Pr$_2$)]$^-$ anion showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 50% probability level. Hydrogen atoms are not shown.

Table 1f. Crystallographic Experimental Details for **7**•0.5C_7H_8.

A. Crystal Data	
formula	$C_{38.50}H_{44}Mn_3NO_{12}P_2$
formula weight	939.51
crystal dimensions (mm)	0.42 × 0.26 × 0.14
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
unit cell parameters[a]	
a (Å)	8.4223 (6)
b (Å)	16.2347 (11)
c (Å)	16.3562 (11)
α (deg)	90.7419 (11)
β (deg)	104.0872 (11)
γ (deg)	96.4207 (11)
V (Å^3)	2153.7 (3)
Z	2
ρ_{calcd} (g cm^{-3})	1.449
μ (mm^{-1})	0.999
B. Data Collection and Refinement Conditions	
diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.3°) (20 s exposures)
data collection 2θ limit (deg)	52.80
total data collected	16679 (–10 ≤ h ≤ 10, –20 ≤ k ≤ 20, –20 ≤ l ≤ 20)
independent reflections	8756 (R_{int} = 0.0206)
number of observed reflections (*NO*)	7276 [$F_o^2 \geq 2\sigma(F_o^2)$]
structure solution method	direct methods (*SIR*97[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.8728–0.6790
data/restraints/parameters	8756 [$F_o^2 \geq -3\sigma(F_o^2)$] / 3[e] / 489
goodness-of-fit (S)[f]	1.086 [$F_o^2 \geq -3\sigma(F_o^2)$]
final R indices[g]	
R_1 [$F_o^2 \geq 2\sigma(F_o^2)$]	0.0406
wR_2 [$F_o^2 \geq -3\sigma(F_o^2)$]	0.1272
largest difference peak and hole	1.305 and –0.870 e Å^{-3}

[a]Obtained from least-squares refinement of 5213 reflections with 5.02° < 2θ < 52.74°.

(continued)

Table 1f. Crystallographic Experimental Details for **7**•0.5C_7H_8. (continued)

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

[c]Altomare, A.; Burla, M. C.; Camalli, M.; Cascarano, G. L.; Giacovazzo, C.; Guagliardi, A.; Moliterni, A. G. G.; Polidori, G.; Spagna, R. *J. Appl. Cryst.* **1999**, *32*, 115–119.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted *R*-factors wR_2 and all goodnesses of fit *S* are based on F_o^2; conventional *R*-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. *R*-factors based on F_o^2 are statistically about twice as large as those based on F_o, and *R*-factors based on ALL data will be even larger.

[e]Distances involving the methyl carbon of the inversion-disordered solvent toluene molecule were given fixed idealized values: d(C10S–C11S) = 1.54 Å; d(C10S···C12S) = d(C10S···C16S) = 2.54 Å. The aromatic ring of this molecule was refined as an idealized regular hexagon, with a fixed C–C bond length of 1.39 Å.

[f]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0732P)^2 + 1.1357P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[g]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2f. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for **7**•0.5C_7H_8.

(a) [{κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}Mn(CO)$_4$]$^+$ atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Mn1	0.20446(4)	0.19359(2)	-0.30918(2)	0.02564(11)*
P1	0.16278(8)	0.23759(4)	-0.18018(4)	0.02829(15)*
O11	-0.0504(3)	0.29216(16)	-0.40703(16)	0.0575(6)*
O12	0.2194(3)	0.11665(14)	-0.47379(13)	0.0434(5)*
O13	0.4324(3)	0.34166(13)	-0.32362(16)	0.0505(6)*
O14	0.5146(3)	0.12229(15)	-0.22935(16)	0.0527(6)*
N1	0.0356(3)	0.08380(13)	-0.29701(13)	0.0274(4)*
C1	-0.1296(3)	0.01821(18)	-0.19201(18)	0.0361(6)*
C2	-0.0155(3)	0.08646(16)	-0.21835(16)	0.0279(5)*
C3	0.0305(3)	0.14925(16)	-0.16053(16)	0.0302(5)*
C3A	-0.0479(3)	0.13082(18)	-0.09021(17)	0.0331(6)*
C4	-0.0410(4)	0.1752(2)	-0.01623(19)	0.0436(7)*
C5	-0.1300(4)	0.1402(2)	0.0388(2)	0.0493(8)*
C6	-0.2226(4)	0.0639(2)	0.0203(2)	0.0521(9)*
C7	-0.2293(4)	0.0192(2)	-0.0534(2)	0.0455(7)*
C7A	-0.1421(3)	0.05317(18)	-0.10907(18)	0.0355(6)*
C11	0.0382(4)	0.25203(18)	-0.36761(18)	0.0363(6)*
C12	0.2167(3)	0.14660(17)	-0.41120(18)	0.0324(6)*
C13	0.3444(4)	0.28479(17)	-0.31772(18)	0.0343(6)*
C14	0.3936(3)	0.14555(17)	-0.25619(18)	0.0337(6)*
C21	0.0470(4)	0.32718(19)	-0.1727(2)	0.0438(7)*
C22	-0.1369(4)	0.3090(2)	-0.2121(3)	0.0584(9)*
C23	0.1201(5)	0.4054(2)	-0.2074(3)	0.0613(10)*
C24	0.3388(4)	0.2536(2)	-0.08562(18)	0.0419(7)*
C25	0.4879(4)	0.3066(3)	-0.1036(2)	0.0583(10)*
C26	0.3880(4)	0.1732(3)	-0.0475(2)	0.0593(10)*
C27	-0.1167(3)	0.0754(2)	-0.36798(18)	0.0408(7)*
C28	0.1160(4)	0.00625(17)	-0.2998(2)	0.0431(7)*

(b) [Mn_2(CO)$_8$(μ–P^iPr_2)]$^-$ atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Mn2	0.55412(4)	0.18194(2)	0.39609(2)	0.02567(11)*
Mn3	0.56832(5)	0.25152(3)	0.23877(3)	0.03575(12)*
P2	0.54818(8)	0.31600(4)	0.35829(4)	0.02802(15)*
O31	0.1884(2)	0.15381(13)	0.33993(14)	0.0431(5)*
O32	0.5381(3)	-0.00045(14)	0.3779(2)	0.0650(7)*
O33	0.5703(3)	0.20476(14)	0.57659(12)	0.0423(5)*
O34	0.9183(3)	0.18912(17)	0.43270(15)	0.0545(6)*
O35	0.2059(3)	0.2229(2)	0.17028(16)	0.0662(7)*

Table 2f. Atomic Coordinates and Displacement Parameters for **7**•0.5C_7H_8. (continued)

(b) [$Mn_2(CO)_8(\mu$–$P^iPr_2)$]$^-$ atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
O36	0.5890(4)	0.08214(19)	0.17605(17)	0.0738(8)*
O37	0.5601(4)	0.3682(2)	0.10265(19)	0.0893(10)*
O38	0.9312(3)	0.2964(2)	0.27730(19)	0.0820(10)*
C31	0.3293(3)	0.16686(16)	0.36078(17)	0.0298(5)*
C32	0.5464(3)	0.07092(19)	0.3837(2)	0.0390(6)*
C33	0.5610(3)	0.19519(17)	0.50517(17)	0.0311(6)*
C34	0.7783(3)	0.18919(18)	0.41621(17)	0.0346(6)*
C35	0.3452(4)	0.2339(2)	0.20015(18)	0.0425(7)*
C36	0.5838(4)	0.1483(3)	0.2004(2)	0.0513(8)*
C37	0.5648(4)	0.3217(3)	0.1563(2)	0.0552(9)*
C38	0.7929(4)	0.2774(3)	0.2665(2)	0.0523(9)*
C41	0.3530(4)	0.36062(17)	0.35697(19)	0.0359(6)*
C42	0.2970(4)	0.35552(19)	0.4396(2)	0.0418(7)*
C43	0.3483(5)	0.4479(2)	0.3223(2)	0.0542(9)*
C44	0.7273(4)	0.39047(18)	0.4152(2)	0.0424(7)*
C45	0.7133(4)	0.4204(2)	0.5015(2)	0.0515(8)*
C46	0.7706(5)	0.4630(2)	0.3630(3)	0.0664(11)*

(c) solvent toluene atoms

Atom	*x*	*y*	*z*	U_{eq}, Å^2
C10S[a]	-0.1346(12)	0.5811(8)	-0.0888(9)	0.1187(14)
C11S[a]	-0.0355(9)	0.5236(7)	-0.0272(8)	0.1187(14)
C12S[a]	0.1344(9)	0.5282(6)	-0.0155(7)	0.1187(14)
C13S[a]	0.2231(9)	0.4744(6)	0.0379(6)	0.1187(14)
C14S[a]	0.1420(11)	0.4160(6)	0.0796(7)	0.1187(14)
C15S[a]	-0.0279(11)	0.4114(6)	0.0680(6)	0.1187(14)
C16S[a]	-0.1166(9)	0.4652(6)	0.0146(7)	0.1187(14)

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$. [a]Atoms of the solvent toluene molecule were refined with an occupancy factor of 0.5 and a common isotropic displacement parameter.

Table 3f. Selected Interatomic Distances (Å) for **7**•0.5C_7H_8.

(a) within [{κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}Mn(CO)$_4$]$^+$

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Mn1	P1	2.3373(8)	N1	C28	1.500(3)
Mn1	N1	2.195(2)	C1	C2	1.521(3)
Mn1	C11	1.856(3)	C1	C7A	1.495(4)
Mn1	C12	1.856(3)	C2	C3	1.339(4)
Mn1	C13	1.816(3)	C3	C3A	1.478(4)
Mn1	C14	1.877(3)	C3A	C4	1.385(4)
P1	C3	1.797(3)	C3A	C7A	1.400(4)
P1	C21	1.858(3)	C4	C5	1.393(4)
P1	C24	1.856(3)	C5	C6	1.377(5)
O11	C11	1.132(4)	C6	C7	1.385(5)
O12	C12	1.134(3)	C7	C7A	1.387(4)
O13	C13	1.138(3)	C21	C22	1.519(5)
O14	C14	1.116(3)	C21	C23	1.526(4)
N1	C2	1.454(3)	C24	C25	1.532(4)
N1	C27	1.498(3)	C24	C26	1.510(5)

(b) within [Mn_2(CO)$_8$(μ–P^iPr_2)]$^-$

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Mn2	Mn3	2.8472(6)	O31	C31	1.146(3)
Mn2	P2	2.2728(8)	O32	C32	1.154(4)
Mn2	C31	1.828(3)	O33	C33	1.159(3)
Mn2	C32	1.803(3)	O34	C34	1.144(3)
Mn2	C33	1.780(3)	O35	C35	1.148(4)
Mn2	C34	1.826(3)	O36	C36	1.149(4)
Mn3	P2	2.2571(8)	O37	C37	1.161(4)
Mn3	C35	1.819(3)	O38	C38	1.141(4)
Mn3	C36	1.812(4)	C41	C42	1.536(4)
Mn3	C37	1.773(4)	C41	C43	1.534(4)
Mn3	C38	1.833(3)	C44	C45	1.523(5)
P2	C41	1.865(3)	C44	C46	1.526(5)
P2	C44	1.866(3)			

(c) within the solvent toluene molecule

Atom1	Atom2	Distance	Atom1	Atom2	Distance
C10S	C11S	1.54†	C13S	C14S	1.39†
C11S	C12S	1.39†	C14S	C15S	1.39†
C11S	C16S	1.39†	C15S	C16S	1.39†
C12S	C13S	1.39†			

†Distance fixed during refinement.

Table 4f. Selected Interatomic Angles (deg) for **7**•0.5C_7H_8.

(a) within [{κ²–(2-Me_2N-1H-inden-3-yl)P^iPr_2}Mn(CO)$_4$]$^+$

Atom1	Atom2	Distance		Atom1	Atom2	Distance	
P1	Mn1	N1	84.59(6)	C2	C1	C7A	101.4(2)
P1	Mn1	C11	91.02(9)	N1	C2	C1	124.0(2)
P1	Mn1	C12	172.31(8)	N1	C2	C3	124.5(2)
P1	Mn1	C13	94.63(9)	C1	C2	C3	111.6(2)
P1	Mn1	C14	92.30(9)	P1	C3	C2	118.9(2)
N1	Mn1	C11	94.29(11)	P1	C3	C3A	132.0(2)
N1	Mn1	C12	87.74(10)	C2	C3	C3A	109.1(2)
N1	Mn1	C13	179.20(10)	C3	C3A	C4	131.8(3)
N1	Mn1	C14	93.69(10)	C3	C3A	C7A	107.3(2)
C11	Mn1	C12	88.97(12)	C4	C3A	C7A	120.8(3)
C11	Mn1	C13	85.90(13)	C3A	C4	C5	118.1(3)
C11	Mn1	C14	171.61(12)	C4	C5	C6	121.1(3)
C12	Mn1	C13	93.04(12)	C5	C6	C7	121.0(3)
C12	Mn1	C14	88.76(12)	C6	C7	C7A	118.7(3)
C13	Mn1	C14	86.15(12)	C1	C7A	C3A	110.6(2)
Mn1	P1	C3	99.78(9)	C1	C7A	C7	129.1(3)
Mn1	P1	C21	121.13(10)	C3A	C7A	C7	120.3(3)
Mn1	P1	C24	120.01(10)	Mn1	C11	O11	172.4(3)
C3	P1	C21	104.38(13)	Mn1	C12	O12	177.9(2)
C3	P1	C24	106.12(13)	Mn1	C13	O13	179.4(3)
C21	P1	C24	103.38(16)	Mn1	C14	O14	172.8(3)
Mn1	N1	C2	112.23(15)	P1	C21	C22	113.5(2)
Mn1	N1	C27	111.26(16)	P1	C21	C23	112.2(2)
Mn1	N1	C28	110.62(16)	C22	C21	C23	111.0(3)
C2	N1	C27	107.8(2)	P1	C24	C25	112.1(2)
C2	N1	C28	107.7(2)	P1	C24	C26	112.8(2)
C27	N1	C28	107.0(2)	C25	C24	C26	110.7(3)

(b) within [Mn_2(CO)$_8$(μ–P^iPr_2)]$^-$

Atom1	Atom2	Distance		Atom1	Atom2	Distance	
Mn3	Mn2	P2	50.81(2)	C31	Mn2	C32	86.84(12)
Mn3	Mn2	C31	89.37(8)	C31	Mn2	C33	95.44(12)
Mn3	Mn2	C32	107.97(10)	C31	Mn2	C34	171.33(12)
Mn3	Mn2	C33	149.91(9)	C32	Mn2	C33	101.96(13)
Mn3	Mn2	C34	85.10(9)	C32	Mn2	C34	88.51(13)
P2	Mn2	C31	88.61(8)	C33	Mn2	C34	92.68(12)
P2	Mn2	C32	158.37(10)	Mn2	Mn3	P2	51.31(2)
P2	Mn2	C33	99.51(9)	Mn2	Mn3	C35	91.77(10)
P2	Mn2	C34	93.05(9)	Mn2	Mn3	C36	87.75(11)

Table 4f. Selected Interatomic Angles for **7**•0.5C_7H_8. (continued)

(b) within [$Mn_2(CO)_8(\mu$–$P^iPr_2)]^-$

Atom1	Atom2	Distance		Atom1	Atom2	Distance	
Mn2	Mn3	C37	162.66(13)	Mn3	P2	C44	117.61(11)
Mn2	Mn3	C38	95.17(10)	C41	P2	C44	109.34(14)
P2	Mn3	C35	91.62(10)	Mn2	C31	O31	176.9(2)
P2	Mn3	C36	139.05(11)	Mn2	C32	O32	177.6(3)
P2	Mn3	C37	111.47(13)	Mn2	C33	O33	178.0(2)
P2	Mn3	C38	91.48(11)	Mn2	C34	O34	175.0(3)
C35	Mn3	C36	90.03(15)	Mn3	C35	O35	175.3(3)
C35	Mn3	C37	86.40(16)	Mn3	C36	O36	178.0(3)
C35	Mn3	C38	172.87(15)	Mn3	C37	O37	178.8(4)
C36	Mn3	C37	109.47(17)	Mn3	C38	O38	174.3(3)
C36	Mn3	C38	91.84(17)	P2	C41	C42	115.5(2)
C37	Mn3	C38	86.49(16)	P2	C41	C43	113.6(2)
Mn2	P2	Mn3	77.88(3)	C42	C41	C43	111.6(3)
Mn2	P2	C41	115.66(9)	P2	C44	C45	113.6(2)
Mn2	P2	C44	115.74(10)	P2	C44	C46	114.1(2)
Mn3	P2	C41	117.82(10)	C45	C44	C46	111.3(3)

(c) within the solvent toluene molecule

Atom1	Atom2	Distance		Atom1	Atom2	Distance	
C10S	C11S	C12S	120.0†	C12S	C13S	C14S	120.0†
C10S	C11S	C16S	120.0†	C13S	C14S	C15S	120.0†
C12S	C11S	C16S	120.0†	C14S	C15S	C16S	120.0†
C11S	C12S	C13S	120.0†	C11S	C16S	C15S	120.0†

†Angle fixed during refinement.

Table 5f. Torsional Angles (deg) for **7**•0.5C_7H_8.

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
N1	Mn1	P1	C3	2.35(10)	P1	Mn1	C13	O13	172(100)
N1	Mn1	P1	C21	-111.14(14)	N1	Mn1	C13	O13	159(33)
N1	Mn1	P1	C24	117.49(13)	C11	Mn1	C13	O13	-97(37)
C11	Mn1	P1	C3	96.56(13)	C12	Mn1	C13	O13	-8(37)
C11	Mn1	P1	C21	-16.92(15)	C14	Mn1	C13	O13	80(37)
C11	Mn1	P1	C24	-148.30(15)	P1	Mn1	C14	O14	-122(2)
C12	Mn1	P1	C3	6.7(7)	N1	Mn1	C14	O14	154(2)
C12	Mn1	P1	C21	-106.8(7)	C11	Mn1	C14	O14	-8(3)
C12	Mn1	P1	C24	121.8(7)	C12	Mn1	C14	O14	66(2)
C13	Mn1	P1	C3	-177.47(12)	C13	Mn1	C14	O14	-27(2)
C13	Mn1	P1	C21	69.05(15)	Mn1	P1	C3	C2	-2.4(2)
C13	Mn1	P1	C24	-62.33(15)	Mn1	P1	C3	C3A	179.8(2)
C14	Mn1	P1	C3	-91.15(12)	C21	P1	C3	C2	123.5(2)
C14	Mn1	P1	C21	155.37(15)	C21	P1	C3	C3A	-54.3(3)
C14	Mn1	P1	C24	24.00(15)	C24	P1	C3	C2	-127.7(2)
P1	Mn1	N1	C2	-2.47(15)	C24	P1	C3	C3A	54.5(3)
P1	Mn1	N1	C27	118.41(18)	Mn1	P1	C21	C22	71.3(2)
P1	Mn1	N1	C28	-122.80(19)	Mn1	P1	C21	C23	-55.6(3)
C11	Mn1	N1	C2	-93.09(18)	C3	P1	C21	C22	-39.8(3)
C11	Mn1	N1	C27	27.8(2)	C3	P1	C21	C23	-166.7(3)
C11	Mn1	N1	C28	146.6(2)	C24	P1	C21	C22	-150.6(2)
C12	Mn1	N1	C2	178.11(18)	C24	P1	C21	C23	82.5(3)
C12	Mn1	N1	C27	-61.01(19)	Mn1	P1	C24	C25	49.2(3)
C12	Mn1	N1	C28	57.8(2)	Mn1	P1	C24	C26	-76.5(2)
C13	Mn1	N1	C2	11(8)	C3	P1	C24	C25	161.0(3)
C13	Mn1	N1	C27	132(8)	C3	P1	C24	C26	35.3(3)
C13	Mn1	N1	C28	-110(8)	C21	P1	C24	C25	-89.4(3)
C14	Mn1	N1	C2	89.50(18)	C21	P1	C24	C26	144.9(2)
C14	Mn1	N1	C27	-149.62(19)	Mn1	N1	C2	C1	-178.8(2)
C14	Mn1	N1	C28	-30.8(2)	Mn1	N1	C2	C3	1.7(3)
P1	Mn1	C11	O11	122(2)	C27	N1	C2	C1	58.3(3)
N1	Mn1	C11	O11	-153(2)	C27	N1	C2	C3	-121.1(3)
C12	Mn1	C11	O11	-66(2)	C28	N1	C2	C1	-56.8(3)
C13	Mn1	C11	O11	27(2)	C28	N1	C2	C3	123.7(3)
C14	Mn1	C11	O11	9(3)	C7A	C1	C2	N1	-179.1(2)
P1	Mn1	C12	O12	24(8)	C7A	C1	C2	C3	0.4(3)
N1	Mn1	C12	O12	28(7)	C2	C1	C7A	C3A	-0.1(3)
C11	Mn1	C12	O12	-66(7)	C2	C1	C7A	C7	-179.7(3)
C13	Mn1	C12	O12	-152(7)	N1	C2	C3	P1	0.6(4)
C14	Mn1	C12	O12	122(7)	N1	C2	C3	C3A	178.9(2)

Table 5f. Torsional Angles for **7**•0.5C_7H_8. (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C1	C2	C3	P1	-178.83(18)	C34	Mn2	Mn3	C38	-10.23(16)
C1	C2	C3	C3A	-0.6(3)	Mn3	Mn2	P2	C41	115.24(11)
P1	C3	C3A	C4	-1.7(5)	Mn3	Mn2	P2	C44	-115.00(12)
P1	C3	C3A	C7A	178.4(2)	C31	Mn2	P2	Mn3	-90.33(8)
C2	C3	C3A	C4	-179.7(3)	C31	Mn2	P2	C41	24.92(13)
C2	C3	C3A	C7A	0.5(3)	C31	Mn2	P2	C44	154.67(15)
C3	C3A	C4	C5	-179.6(3)	C32	Mn2	P2	Mn3	-12.5(3)
C7A	C3A	C4	C5	0.2(5)	C32	Mn2	P2	C41	102.7(3)
C3	C3A	C7A	C1	-0.2(3)	C32	Mn2	P2	C44	-127.5(3)
C3	C3A	C7A	C7	179.4(3)	C33	Mn2	P2	Mn3	174.39(8)
C4	C3A	C7A	C1	179.9(3)	C33	Mn2	P2	C41	-70.37(13)
C4	C3A	C7A	C7	-0.5(4)	C33	Mn2	P2	C44	59.39(15)
C3A	C4	C5	C6	-0.2(5)	C34	Mn2	P2	Mn3	81.16(9)
C4	C5	C6	C7	0.5(5)	C34	Mn2	P2	C41	-163.60(14)
C5	C6	C7	C7A	-0.8(5)	C34	Mn2	P2	C44	-33.85(15)
C6	C7	C7A	C1	-179.7(3)	Mn3	Mn2	C31	O31	133(5)
C6	C7	C7A	C3A	0.7(5)	P2	Mn2	C31	O31	-176(100)
P2	Mn2	Mn3	C35	-90.66(11)	C32	Mn2	C31	O31	25(5)
P2	Mn2	Mn3	C36	179.38(12)	C33	Mn2	C31	O31	-76(5)
P2	Mn2	Mn3	C37	-7.1(4)	C34	Mn2	C31	O31	83(5)
P2	Mn2	Mn3	C38	87.74(13)	Mn3	Mn2	C32	O32	-148(7)
C31	Mn2	Mn3	P2	88.71(8)	P2	Mn2	C32	O32	-138(7)
C31	Mn2	Mn3	C35	-1.95(13)	C31	Mn2	C32	O32	-60(7)
C31	Mn2	Mn3	C36	-91.90(14)	C33	Mn2	C32	O32	35(7)
C31	Mn2	Mn3	C37	81.6(4)	C34	Mn2	C32	O32	127(7)
C31	Mn2	Mn3	C38	176.46(15)	Mn3	Mn2	C33	O33	-66(7)
C32	Mn2	Mn3	P2	175.19(10)	P2	Mn2	C33	O33	-75(7)
C32	Mn2	Mn3	C35	84.53(14)	C31	Mn2	C33	O33	-165(7)
C32	Mn2	Mn3	C36	-5.43(14)	C32	Mn2	C33	O33	107(7)
C32	Mn2	Mn3	C37	168.1(4)	C34	Mn2	C33	O33	18(7)
C32	Mn2	Mn3	C38	-97.07(16)	Mn3	Mn2	C34	O34	-154(3)
C33	Mn2	Mn3	P2	-11.09(17)	P2	Mn2	C34	O34	155(3)
C33	Mn2	Mn3	C35	-101.7(2)	C31	Mn2	C34	O34	-104(3)
C33	Mn2	Mn3	C36	168.3(2)	C32	Mn2	C34	O34	-46(3)
C33	Mn2	Mn3	C37	-18.2(4)	C33	Mn2	C34	O34	56(3)
C33	Mn2	Mn3	C38	76.7(2)	Mn2	Mn3	P2	C41	-112.80(11)
C34	Mn2	Mn3	P2	-97.98(9)	Mn2	Mn3	P2	C44	112.90(12)
C34	Mn2	Mn3	C35	171.36(14)	C35	Mn3	P2	Mn2	90.97(11)
C34	Mn2	Mn3	C36	81.41(14)	C35	Mn3	P2	C41	-21.82(15)
C34	Mn2	Mn3	C37	-105.1(4)	C35	Mn3	P2	C44	-156.13(15)

Table 5f. Torsional Angles for **7**•0.5C_7H_8. (continued)

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C36	Mn3	P2	Mn2	-0.94(18)	P2	Mn3	C38	O38	-126(4)
C36	Mn3	P2	C41	-113.7(2)	C35	Mn3	C38	O38	-10(5)
C36	Mn3	P2	C44	112.0(2)	C36	Mn3	C38	O38	95(4)
C37	Mn3	P2	Mn2	177.74(13)	C37	Mn3	C38	O38	-15(4)
C37	Mn3	P2	C41	64.94(17)	Mn2	P2	C41	C42	55.2(2)
C37	Mn3	P2	C44	-69.37(17)	Mn2	P2	C41	C43	-174.0(2)
C38	Mn3	P2	Mn2	-95.45(12)	Mn3	P2	C41	C42	144.59(18)
C38	Mn3	P2	C41	151.76(16)	Mn3	P2	C41	C43	-84.5(2)
C38	Mn3	P2	C44	17.45(17)	C44	P2	C41	C42	-77.6(2)
Mn2	Mn3	C35	O35	-156(4)	C44	P2	C41	C43	53.2(3)
P2	Mn3	C35	O35	152(4)	Mn2	P2	C44	C45	-81.6(2)
C36	Mn3	C35	O35	-69(4)	Mn2	P2	C44	C46	149.3(2)
C37	Mn3	C35	O35	41(4)	Mn3	P2	C44	C45	-171.00(19)
C38	Mn3	C35	O35	37(5)	Mn3	P2	C44	C46	59.9(3)
Mn2	Mn3	C36	O36	70(9)	C41	P2	C44	C45	51.1(3)
P2	Mn3	C36	O36	71(9)	C41	P2	C44	C46	-77.9(3)
C35	Mn3	C36	O36	-21(9)	C10S	C11S	C12S	C13S	-177.9(15)
C37	Mn3	C36	O36	-108(9)	C16S	C11S	C12S	C13S	0.0†
C38	Mn3	C36	O36	165(9)	C10S	C11S	C16S	C15S	177.8(15)
Mn2	Mn3	C37	O37	-45(20)	C12S	C11S	C16S	C15S	0.0†
P2	Mn3	C37	O37	-50(19)	C11S	C12S	C13S	C14S	0.0†
C35	Mn3	C37	O37	40(19)	C12S	C13S	C14S	C15S	0.0†
C36	Mn3	C37	O37	129(19)	C13S	C14S	C15S	C16S	0.0†
C38	Mn3	C37	O37	-141(19)	C14S	C15S	C16S	C11S	0.0†
Mn2	Mn3	C38	O38	-177(100)					

†Angle fixed during refinement.

Table 6f. Least-Squares Planes for **7**•0.5C_7H_8.

Plane	Coefficients[a]				Defining Atoms with Deviations (Å)[b]			
1	-6.354(5)	8.832(15)	-4.685(10)	1.8820(15)				
					C1	0.002(2)	C2	0.003(2)
					C3	-0.006(2)	C3A	0.000(3)
					C4	0.002(3)	C5	0.001(3)
					C6	0.002(3)	C7	-0.006(3)
					C7A	0.002(3)		
					<u>P1</u>	0.026(3)	<u>N1</u>	0.024(3)

[a]Coefficients are for the form $ax+by+cz = d$ where x, y and z are crystallographic coordinates.
[b]Underlined atoms were not included in the definition of the plane.

Table 7f. Anisotropic Displacement Parameters (U_{ij}, Å^2) for **7**•0.5C_7H_8.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mn1	0.0249(2)	0.0257(2)	0.0272(2)	0.00357(15)	0.00794(15)	0.00316(15)
P1	0.0288(3)	0.0278(3)	0.0283(3)	0.0009(3)	0.0094(3)	-0.0018(3)
O11	0.0606(15)	0.0569(14)	0.0518(14)	0.0081(12)	-0.0017(12)	0.0272(12)
O12	0.0434(12)	0.0544(13)	0.0349(11)	-0.0047(10)	0.0147(9)	0.0065(10)
O13	0.0575(14)	0.0347(11)	0.0642(15)	0.0040(10)	0.0298(12)	-0.0066(10)
O14	0.0399(12)	0.0528(14)	0.0611(15)	-0.0012(11)	-0.0007(11)	0.0177(10)
N1	0.0256(10)	0.0270(11)	0.0291(11)	0.0009(9)	0.0064(9)	0.0010(8)
C1	0.0330(14)	0.0335(14)	0.0385(15)	0.0075(12)	0.0062(12)	-0.0048(11)
C2	0.0230(11)	0.0286(13)	0.0315(13)	0.0080(10)	0.0057(10)	0.0020(10)
C3	0.0261(12)	0.0332(14)	0.0304(13)	0.0059(11)	0.0065(10)	0.0001(10)
C3A	0.0276(13)	0.0406(15)	0.0298(13)	0.0074(11)	0.0065(10)	-0.0003(11)
C4	0.0401(16)	0.0561(19)	0.0332(15)	0.0019(13)	0.0111(12)	-0.0045(14)
C5	0.0449(17)	0.072(2)	0.0329(16)	0.0029(15)	0.0153(13)	0.0023(16)
C6	0.0412(17)	0.074(2)	0.0430(18)	0.0193(17)	0.0172(14)	-0.0038(16)
C7	0.0408(16)	0.0544(19)	0.0400(17)	0.0133(14)	0.0131(13)	-0.0081(14)
C7A	0.0282(13)	0.0422(15)	0.0333(14)	0.0100(12)	0.0044(11)	-0.0013(11)
C11	0.0382(15)	0.0361(15)	0.0351(15)	0.0006(12)	0.0090(12)	0.0069(12)
C12	0.0277(13)	0.0330(14)	0.0371(15)	0.0062(12)	0.0095(11)	0.0021(10)
C13	0.0389(15)	0.0308(14)	0.0360(15)	0.0035(11)	0.0144(12)	0.0049(12)
C14	0.0306(14)	0.0308(14)	0.0379(15)	-0.0015(11)	0.0062(11)	0.0019(11)
C21	0.060(2)	0.0354(15)	0.0451(17)	0.0003(13)	0.0286(15)	0.0113(14)
C22	0.054(2)	0.059(2)	0.076(3)	0.0179(19)	0.0327(19)	0.0263(17)
C23	0.079(3)	0.0332(17)	0.080(3)	0.0029(17)	0.034(2)	0.0077(17)
C24	0.0347(15)	0.0564(19)	0.0297(14)	-0.0049(13)	0.0061(12)	-0.0113(13)
C25	0.0453(19)	0.070(2)	0.051(2)	-0.0077(17)	0.0089(15)	-0.0243(17)
C26	0.0412(18)	0.084(3)	0.0437(19)	0.0191(18)	-0.0041(14)	-0.0018(17)
C27	0.0328(14)	0.0536(18)	0.0303(14)	0.0020(13)	0.0024(11)	-0.0065(13)
C28	0.0417(16)	0.0251(14)	0.067(2)	0.0008(13)	0.0236(15)	0.0021(12)
Mn2	0.0249(2)	0.0269(2)	0.0260(2)	-0.00036(15)	0.00779(15)	0.00327(15)
Mn3	0.0322(2)	0.0524(3)	0.0241(2)	0.00424(18)	0.00828(17)	0.00818(19)
P2	0.0268(3)	0.0282(3)	0.0274(3)	0.0021(3)	0.0048(3)	-0.0003(3)
O31	0.0311(11)	0.0409(11)	0.0543(13)	-0.0005(10)	0.0086(9)	-0.0038(9)
O32	0.0574(15)	0.0302(12)	0.110(2)	-0.0092(13)	0.0247(15)	0.0084(10)
O33	0.0414(11)	0.0582(13)	0.0284(11)	-0.0005(9)	0.0107(8)	0.0055(10)
O34	0.0301(11)	0.0844(18)	0.0515(14)	0.0070(12)	0.0101(10)	0.0162(11)
O35	0.0405(14)	0.103(2)	0.0451(14)	-0.0057(14)	-0.0057(11)	0.0005(13)
O36	0.096(2)	0.078(2)	0.0506(15)	-0.0135(14)	0.0091(14)	0.0435(17)
O37	0.100(2)	0.113(3)	0.0572(18)	0.0447(18)	0.0225(16)	0.010(2)
O38	0.0350(14)	0.139(3)	0.0748(19)	0.0252(19)	0.0204(13)	0.0060(15)
C31	0.0326(14)	0.0243(12)	0.0321(13)	-0.0017(10)	0.0089(11)	-0.0004(10)

Table 7f. Anisotropic Displacement Parameters for **7**•0.5C_7H_8. (continued)

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C32	0.0323(14)	0.0377(16)	0.0488(17)	-0.0038(13)	0.0122(12)	0.0071(12)
C33	0.0254(12)	0.0331(14)	0.0352(15)	0.0002(11)	0.0090(10)	0.0027(10)
C34	0.0335(15)	0.0419(16)	0.0305(14)	0.0031(12)	0.0102(11)	0.0081(12)
C35	0.0429(17)	0.0562(19)	0.0261(14)	-0.0027(13)	0.0039(12)	0.0068(14)
C36	0.0520(19)	0.072(2)	0.0308(16)	0.0014(16)	0.0062(14)	0.0218(17)
C37	0.052(2)	0.080(3)	0.0350(17)	0.0110(17)	0.0129(15)	0.0065(18)
C38	0.0407(18)	0.083(3)	0.0370(17)	0.0125(16)	0.0151(14)	0.0094(17)
C41	0.0361(14)	0.0305(14)	0.0408(16)	-0.0006(11)	0.0072(12)	0.0089(11)
C42	0.0458(17)	0.0343(15)	0.0488(18)	-0.0031(13)	0.0168(14)	0.0095(13)
C43	0.062(2)	0.0427(18)	0.059(2)	0.0129(16)	0.0111(17)	0.0195(16)
C44	0.0357(15)	0.0327(15)	0.0508(18)	0.0039(13)	-0.0016(13)	-0.0033(12)
C45	0.0491(18)	0.0363(16)	0.057(2)	-0.0125(15)	-0.0088(15)	0.0048(14)
C46	0.049(2)	0.049(2)	0.091(3)	0.019(2)	0.0076(19)	-0.0191(16)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table 8f. Derived Atomic Coordinates and Displacement Parameters for H-Atoms for **7**•0.5C_7H_8.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1A	-0.2386	0.0095	-0.2330	0.043
H1B	-0.0809	-0.0348	-0.1855	0.043
H4	0.0226	0.2279	-0.0034	0.052
H5	-0.1267	0.1696	0.0900	0.059
H6	-0.2829	0.0416	0.0587	0.063
H7	-0.2924	-0.0338	-0.0655	0.055
H21	0.0596	0.3394	-0.1112	0.053
H22A	-0.1906	0.3584	-0.2059	0.070
H22B	-0.1835	0.2630	-0.1836	0.070
H22C	-0.1552	0.2937	-0.2721	0.070
H23A	0.0557	0.4510	-0.2021	0.074
H23B	0.1170	0.3952	-0.2670	0.074
H23C	0.2345	0.4203	-0.1754	0.074
H24	0.3018	0.2852	-0.0422	0.050
H25A	0.5775	0.3139	-0.0522	0.070
H25B	0.4566	0.3610	-0.1222	0.070
H25C	0.5249	0.2788	-0.1480	0.070
H26A	0.4807	0.1852	0.0022	0.071
H26B	0.4210	0.1393	-0.0891	0.071
H26C	0.2944	0.1430	-0.0307	0.071
H27A	-0.1897	0.0261	-0.3609	0.049
H27B	-0.0862	0.0699	-0.4217	0.049
H27C	-0.1739	0.1248	-0.3678	0.049
H28A	0.0389	-0.0420	-0.2943	0.052
H28B	0.2151	0.0088	-0.2532	0.052
H28C	0.1465	0.0014	-0.3536	0.052
H41	0.2657	0.3246	0.3151	0.043
H42A	0.1939	0.3803	0.4326	0.050
H42B	0.3821	0.3857	0.4851	0.050
H42C	0.2794	0.2973	0.4537	0.050
H43A	0.2428	0.4675	0.3232	0.065
H43B	0.3602	0.4461	0.2642	0.065
H43C	0.4388	0.4857	0.3574	0.065
H44	0.8245	0.3584	0.4263	0.051
H45A	0.8109	0.4590	0.5279	0.062
H45B	0.7058	0.3728	0.5371	0.062
H45C	0.6143	0.4487	0.4950	0.062
H46A	0.8655	0.4992	0.3967	0.080
H46B	0.6761	0.4946	0.3463	0.080
H46C	0.7981	0.4418	0.3124	0.080

Table 8f. Derived Parameters for Hydrogen Atoms for **7**•0.5C_7H_8. (continued)

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H10A[a]	-0.0589	0.6258	-0.1031	0.142
H10B[a]	-0.2123	0.6051	-0.0622	0.142
H10C[a]	-0.1956	0.5492	-0.1402	0.142
H12S[a]	0.1898	0.5682	-0.0441	0.142
H13S[a]	0.3392	0.4776	0.0458	0.142
H14S[a]	0.2027	0.3793	0.1161	0.142
H15S[a]	-0.0833	0.3715	0.0965	0.142
H16S[a]	-0.2327	0.4620	0.0066	0.142

[a]Included with an occupancy factor of 0.5.

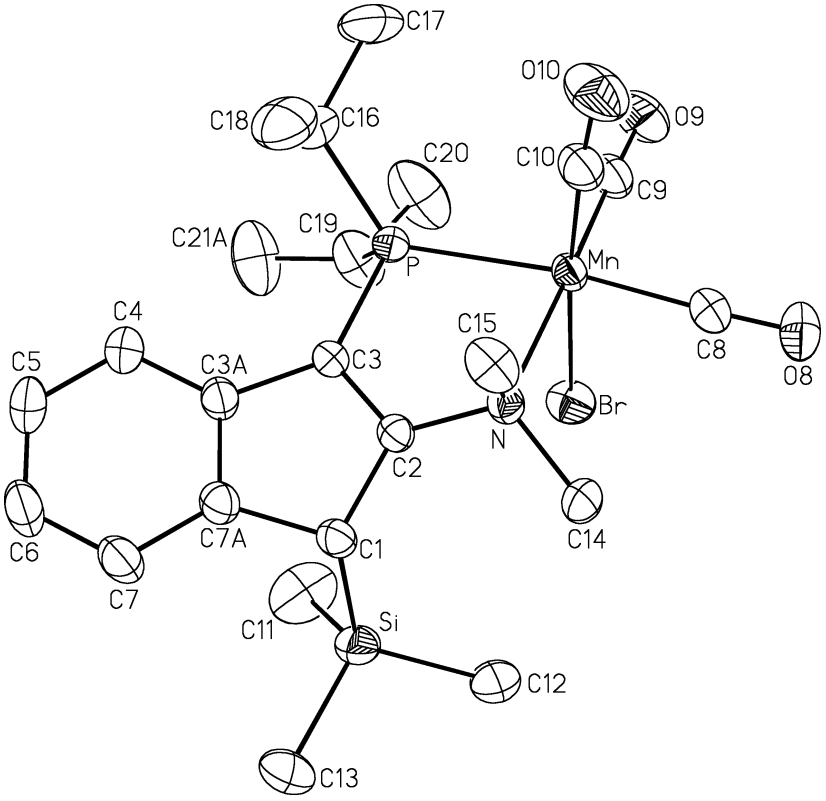

Figure 1g. Perspective view of the [{*N*-(3-(^{i}Pr$_2$P)-1-(Me$_3$Si)-1*H*-inden-2-yl)-*N*,*N*-dimethyl-amino}Mn(CO)$_3$Br] molecule showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 50% probability level. Only the major part of the disorder isopropyl carbon atom (C21A) is shown for clarity. Hydrogen atoms are not shown.

Table 1g. Crystallographic Experimental Details for **10**.

A. Crystal Data	
formula	$C_{23}H_{34}BrMnNO_3PSi$
formula weight	566.42
crystal dimensions (mm)	0.60 × 0.53 × 0.08
crystal system	monoclinic
space group	$P2_1/n$ (an alternate setting of $P2_1/c$ [No. 14])
unit cell parameters[a]	
a (Å)	11.5389 (7)
b (Å)	18.9547 (12)
c (Å)	12.3557 (8)
β (deg)	105.5220 (10)
V (Å^3)	2603.8 (3)
Z	4
ρ_{calcd} (g cm^{-3})	1.445
μ (mm^{-1})	2.173
B. Data Collection and Refinement Conditions	
diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.3°) (25 s exposures)
data collection 2θ limit (deg)	52.76
total data collected	17411 ($-14 \le h \le 14$, $-22 \le k \le 23$, $-15 \le l \le 15$)
independent reflections	5332 (R_{int} = 0.0287)
number of observed reflections (*NO*)	4653 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–86*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	multi-scan (*SADABS*)
range of transmission factors	0.8454–0.3556
data/restraints/parameters	5332 [$F_o^2 \ge -3\sigma(F_o^2)$] / 1[e] / 284
goodness-of-fit (S)[f]	1.023 [$F_o^2 \ge -3\sigma(F_o^2)$]
final R indices[g]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0349
wR_2 [$F_o^2 \ge -3\sigma(F_o^2)$]	0.0946
largest difference peak and hole	0.894 and –0.552 e Å^{-3}

[a]Obtained from least-squares refinement of 5356 reflections with 5.50° < 2θ < 52.72°.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table 1g. Crystallographic Experimental Details for **10**. (continued)

[c]Sheldrick, G. M. *Acta Crystallogr*. **1990**, *A46*, 467–473.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted *R*-factors wR_2 and all goodnesses of fit *S* are based on F_o^2; conventional *R*-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. *R*-factors based on F_o^2 are statistically about twice as large as those based on F_o, and *R*-factors based on ALL data will be even larger.

[e]The C19–C21B distance of the disordered isopropyl group was restrained to be 1.50(1) Å.

[f]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0505P)^2 + 2.3394P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[g]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2g. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for **10**.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Br	0.24795(2)	0.229605(15)	0.40129(2)	0.03745(10)*
Mn	0.30067(3)	0.169119(19)	0.23899(3)	0.02393(10)*
P	0.21010(5)	0.06567(3)	0.28264(5)	0.02622(14)*
Si	-0.15190(7)	0.22566(4)	0.26549(7)	0.03358(17)*
O8	0.4001(2)	0.30826(12)	0.1995(2)	0.0549(6)*
O9	0.54227(18)	0.13584(13)	0.38151(19)	0.0517(6)*
O10	0.3911(2)	0.10884(14)	0.05965(19)	0.0548(6)*
N	0.11591(17)	0.19356(10)	0.13815(16)	0.0240(4)*
C1	-0.1039(2)	0.16844(12)	0.1533(2)	0.0258(5)*
C2	0.0275(2)	0.15259(12)	0.17798(18)	0.0223(4)*
C3	0.0541(2)	0.08766(12)	0.22354(19)	0.0236(5)*
C3A	-0.0596(2)	0.04993(13)	0.2135(2)	0.0282(5)*
C4	-0.0834(3)	-0.01986(15)	0.2341(3)	0.0414(7)*
C5	-0.2020(3)	-0.04208(17)	0.2076(3)	0.0528(8)*
C6	-0.2958(3)	0.00356(17)	0.1608(3)	0.0500(8)*
C7	-0.2725(2)	0.07310(16)	0.1404(2)	0.0392(6)*
C7A	-0.1544(2)	0.09637(13)	0.1660(2)	0.0285(5)*
C8	0.3587(2)	0.25551(15)	0.2118(2)	0.0345(6)*
C9	0.4466(2)	0.14807(15)	0.3280(2)	0.0343(6)*
C10	0.3502(2)	0.13104(15)	0.1265(2)	0.0349(6)*
C11	-0.1219(4)	0.1754(2)	0.3989(3)	0.0642(10)*
C12	-0.0752(3)	0.31285(16)	0.2991(3)	0.0500(8)*
C13	-0.3159(3)	0.24409(19)	0.2075(3)	0.0545(9)*
C14	0.0899(2)	0.27081(13)	0.1333(2)	0.0341(6)*
C15	0.0986(2)	0.17090(16)	0.0184(2)	0.0359(6)*
C16	0.2332(3)	-0.02102(15)	0.2267(3)	0.0443(7)*
C17	0.3675(3)	-0.0396(2)	0.2506(4)	0.0694(11)*
C18	0.1736(3)	-0.02824(19)	0.1035(3)	0.0574(9)*
C19	0.2223(3)	0.0494(2)	0.4351(3)	0.0510(8)*
C20	0.3512(3)	0.0488(3)	0.5077(3)	0.0729(13)*
C21A	0.1527(5)	-0.0084(3)	0.4644(4)	0.0638(15)*,[a]
C21B	0.1232(11)	0.0589(9)	0.4913(13)	0.089(5)[b]

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$. [a]Refined with an occupancy factor of 0.7. [b]Refined with an occupancy factor of 0.3.

Table 3g. Selected Interatomic Distances (Å) for **10**.

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Br	Mn	2.5216(4)	N	C14	1.492(3)
Mn	P	2.3516(7)	N	C15	1.502(3)
Mn	N	2.2114(19)	C1	C2	1.495(3)
Mn	C8	1.834(3)	C1	C7A	1.510(3)
Mn	C9	1.792(3)	C2	C3	1.354(3)
Mn	C10	1.791(3)	C3	C3A	1.469(3)
P	C3	1.801(2)	C3A	C4	1.389(4)
P	C16	1.830(3)	C3A	C7A	1.404(3)
P	C19	1.877(3)	C4	C5	1.385(4)
Si	C1	1.954(3)	C5	C6	1.385(5)
Si	C11	1.855(3)	C6	C7	1.382(4)
Si	C12	1.868(3)	C7	C7A	1.386(3)
Si	C13	1.869(3)	C16	C17	1.538(4)
O8	C8	1.136(3)	C16	C18	1.499(5)
O9	C9	1.149(3)	C19	C20	1.518(4)
O10	C10	1.136(3)	C19	C21A	1.461(6)
N	C2	1.468(3)	C19	C21B	1.50(1)†

†Distance restrained during refinement.

Table 4g. Selected Interatomic Angles (deg) for **10**.

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
Br	Mn	P	88.86(2)	C14	N	C15	105.60(19)
Br	Mn	N	87.22(5)	Si	C1	C2	115.55(16)
Br	Mn	C8	85.27(9)	Si	C1	C7A	103.75(16)
Br	Mn	C9	90.00(9)	C2	C1	C7A	101.26(19)
Br	Mn	C10	174.77(9)	N	C2	C1	125.7(2)
P	Mn	N	83.30(5)	N	C2	C3	121.3(2)
P	Mn	C8	173.26(9)	C1	C2	C3	111.9(2)
P	Mn	C9	94.34(9)	P	C3	C2	118.02(17)
P	Mn	C10	95.50(9)	P	C3	C3A	133.96(18)
N	Mn	C8	93.09(10)	C2	C3	C3A	108.0(2)
N	Mn	C9	176.39(10)	C3	C3A	C4	131.6(2)
N	Mn	C10	96.14(10)	C3	C3A	C7A	108.0(2)
C8	Mn	C9	88.98(12)	C4	C3A	C7A	120.2(2)
C8	Mn	C10	90.54(13)	C3A	C4	C5	118.6(3)
C9	Mn	C10	86.80(12)	C4	C5	C6	121.4(3)
Mn	P	C3	99.86(8)	C5	C6	C7	120.2(3)
Mn	P	C16	122.92(11)	C6	C7	C7A	119.3(3)
Mn	P	C19	116.63(11)	C1	C7A	C3A	109.4(2)
C3	P	C16	106.59(12)	C1	C7A	C7	130.3(2)
C3	P	C19	104.09(13)	C3A	C7A	C7	120.3(2)
C16	P	C19	104.65(17)	Mn	C8	O8	176.3(3)
C1	Si	C11	108.97(14)	Mn	C9	O9	176.9(3)
C1	Si	C12	116.20(13)	Mn	C10	O10	174.2(2)
C1	Si	C13	106.38(14)	P	C16	C17	112.0(2)
C11	Si	C12	106.98(18)	P	C16	C18	113.1(2)
C11	Si	C13	111.45(19)	C17	C16	C18	109.8(3)
C12	Si	C13	106.90(15)	P	C19	C20	113.2(2)
Mn	N	C2	110.61(13)	P	C19	C21A	118.2(3)
Mn	N	C14	112.40(15)	P	C19	C21B	125.7(7)
Mn	N	C15	110.44(15)	C20	C19	C21A	111.4(3)
C2	N	C14	112.47(19)	C20	C19	C21B	118.4(7)
C2	N	C15	104.93(18)				

Table 5g. Torsional Angles (deg) for **10**.

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
Br	Mn	P	C3	77.86(8)	Br	Mn	C10	O10	20(4)
Br	Mn	P	C16	-164.89(12)	P	Mn	C10	O10	-126(3)
Br	Mn	P	C19	-33.46(12)	N	Mn	C10	O10	150(3)
N	Mn	P	C3	-9.47(9)	C8	Mn	C10	O10	57(3)
N	Mn	P	C16	107.78(13)	C9	Mn	C10	O10	-32(3)
N	Mn	P	C19	-120.79(13)	Mn	P	C3	C2	-3.0(2)
C8	Mn	P	C3	48.4(8)	Mn	P	C3	C3A	178.1(2)
C8	Mn	P	C16	165.6(8)	C16	P	C3	C2	-131.9(2)
C8	Mn	P	C19	-62.9(8)	C16	P	C3	C3A	49.2(3)
C9	Mn	P	C3	167.78(12)	C19	P	C3	C2	117.8(2)
C9	Mn	P	C16	-74.97(15)	C19	P	C3	C3A	-61.0(3)
C9	Mn	P	C19	56.46(15)	Mn	P	C16	C17	54.3(3)
C10	Mn	P	C3	-105.03(12)	Mn	P	C16	C18	-70.4(3)
C10	Mn	P	C16	12.22(15)	C3	P	C16	C17	168.2(3)
C10	Mn	P	C19	143.65(15)	C3	P	C16	C18	43.5(3)
Br	Mn	N	C2	-68.27(14)	C19	P	C16	C17	-81.9(3)
Br	Mn	N	C14	58.37(16)	C19	P	C16	C18	153.4(2)
Br	Mn	N	C15	176.01(16)	Mn	P	C19	C20	-56.0(3)
P	Mn	N	C2	20.91(13)	Mn	P	C19	C21A	171.1(3)
P	Mn	N	C14	147.55(16)	Mn	P	C19	C21B	104.8(9)
P	Mn	N	C15	-94.81(16)	C3	P	C19	C20	-164.9(3)
C8	Mn	N	C2	-153.37(16)	C3	P	C19	C21A	62.3(4)
C8	Mn	N	C14	-26.74(18)	C3	P	C19	C21B	-4.1(9)
C8	Mn	N	C15	90.91(18)	C16	P	C19	C20	83.4(3)
C9	Mn	N	C2	-28.5(17)	C16	P	C19	C21A	-49.5(4)
C9	Mn	N	C14	98.1(16)	C16	P	C19	C21B	-115.8(9)
C9	Mn	N	C15	-144.2(16)	C11	Si	C1	C2	-64.8(2)
C10	Mn	N	C2	115.75(16)	C11	Si	C1	C7A	45.0(2)
C10	Mn	N	C14	-117.61(18)	C12	Si	C1	C2	56.0(2)
C10	Mn	N	C15	0.03(18)	C12	Si	C1	C7A	165.91(17)
Br	Mn	C8	O8	79(4)	C13	Si	C1	C2	174.89(19)
P	Mn	C8	O8	109(4)	C13	Si	C1	C7A	-75.25(19)
N	Mn	C8	O8	166(4)	Mn	N	C2	C1	162.23(18)
C9	Mn	C8	O8	-11(4)	Mn	N	C2	C3	-31.1(3)
C10	Mn	C8	O8	-98(4)	C14	N	C2	C1	35.6(3)
Br	Mn	C9	O9	-129(5)	C14	N	C2	C3	-157.7(2)
P	Mn	C9	O9	142(5)	C15	N	C2	C1	-78.7(3)
N	Mn	C9	O9	-169(4)	C15	N	C2	C3	88.0(3)
C8	Mn	C9	O9	-44(5)	Si	C1	C2	N	-93.7(2)
C10	Mn	C9	O9	47(5)	Si	C1	C2	C3	98.6(2)

Table 5g. Torsional Angles for **10**. (continued)

Atom1	Atom2	Atom3	Atom4	Angle
C7A	C1	C2	N	155.0(2)
C7A	C1	C2	C3	-12.8(3)
Si	C1	C7A	C3A	-109.77(19)
Si	C1	C7A	C7	69.2(3)
C2	C1	C7A	C3A	10.3(3)
C2	C1	C7A	C7	-170.7(3)
N	C2	C3	P	22.9(3)
N	C2	C3	C3A	-157.9(2)
C1	C2	C3	P	-168.73(16)
C1	C2	C3	C3A	10.4(3)
P	C3	C3A	C4	-9.7(4)
P	C3	C3A	C7A	175.7(2)
C2	C3	C3A	C4	171.4(3)
C2	C3	C3A	C7A	-3.3(3)
C3	C3A	C4	C5	-174.5(3)
C7A	C3A	C4	C5	-0.4(4)
C3	C3A	C7A	C1	-5.0(3)
C3	C3A	C7A	C7	176.0(2)
C4	C3A	C7A	C1	179.7(2)
C4	C3A	C7A	C7	0.6(4)
C3A	C4	C5	C6	0.4(5)
C4	C5	C6	C7	-0.6(5)
C5	C6	C7	C7A	0.7(5)
C6	C7	C7A	C1	-179.6(3)
C6	C7	C7A	C3A	-0.8(4)

Table 6g. Least-Squares Planes for **10**.

Plane	Coefficients[a]			Defining Atoms with Deviations (Å)[b]			
1	-3.583(14)	4.79(2)	11.937(4)	2.999(2)			
				C3A	0.0016(19)	C4	-0.001(2)
				C5	0.001(3)	C6	-0.002(2)
				C7	0.003(2)	C7A	-0.0028(18)
2	-3.045(16)	4.84(2)	11.947(5)	2.946(2)			
				C1	0.0158(9)	C3	-0.0161(9)
				C3A	0.0270(15)	C7A	-0.0267(15)
				P	0.109(4)	Si	1.780(3)
3	-1.22(3)	7.39(4)	11.241(17)	3.094(4)			
				C1	C2	C3	
				N	-0.253(7)		
4	-3.067(7)	7.289(13)	11.403(4)	3.0431(18)			
				C2	0.0143(9)	C3	-0.0210(14)
				P	0.0141(9)	Mn	-0.0074(5)
5	-2.707(10)	13.95(3)	8.34(2)	3.538(3)			
				C2	N	Mn	

Dihedral angle between planes 1 and 2: 2.79(12)º

Dihedral angle between planes 2 and 3: 11.9(2)º

Dihedral angle between planes 4 and 5: 24.92(19)º

[a]Coefficients are for the form $ax+by+cz = d$ where x, y and z are crystallographic coordinates.
[b]Underlined atoms were not included in the definition of the plane.

Table 7g. Anisotropic Displacement Parameters (U_{ij}, Å^2) for **10**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Br	0.03603(16)	0.04283(17)	0.03178(15)	-0.01360(11)	0.00612(11)	0.00042(11)
Mn	0.01946(18)	0.0258(2)	0.02669(19)	-0.00240(14)	0.00650(14)	-0.00261(13)
P	0.0206(3)	0.0226(3)	0.0339(3)	0.0017(2)	0.0047(2)	0.0015(2)
Si	0.0329(4)	0.0312(4)	0.0402(4)	-0.0002(3)	0.0158(3)	0.0048(3)
O8	0.0448(12)	0.0390(12)	0.0830(17)	0.0075(11)	0.0206(12)	-0.0119(10)
O9	0.0255(10)	0.0698(16)	0.0545(13)	0.0034(11)	0.0013(9)	0.0026(10)
O10	0.0498(13)	0.0747(16)	0.0487(12)	-0.0131(12)	0.0287(11)	-0.0021(11)
N	0.0230(9)	0.0246(10)	0.0248(10)	0.0027(8)	0.0067(8)	-0.0015(8)
C1	0.0204(11)	0.0277(12)	0.0282(12)	0.0035(9)	0.0047(9)	0.0014(9)
C2	0.0211(11)	0.0239(11)	0.0220(10)	-0.0029(9)	0.0061(8)	-0.0015(9)
C3	0.0199(11)	0.0235(11)	0.0271(11)	-0.0005(9)	0.0057(9)	-0.0002(9)
C3A	0.0254(12)	0.0284(13)	0.0309(12)	-0.0025(10)	0.0082(9)	-0.0041(10)
C4	0.0344(14)	0.0282(14)	0.0632(19)	0.0008(13)	0.0159(13)	-0.0051(11)
C5	0.0452(18)	0.0332(16)	0.084(2)	-0.0069(16)	0.0240(16)	-0.0168(13)
C6	0.0318(15)	0.0483(18)	0.073(2)	-0.0162(16)	0.0192(14)	-0.0166(13)
C7	0.0240(13)	0.0447(16)	0.0479(16)	-0.0094(13)	0.0081(11)	-0.0036(11)
C7A	0.0254(12)	0.0298(13)	0.0304(12)	-0.0064(10)	0.0073(9)	-0.0029(10)
C8	0.0254(12)	0.0360(15)	0.0430(15)	0.0012(12)	0.0106(11)	-0.0028(11)
C9	0.0257(13)	0.0394(15)	0.0378(14)	-0.0040(11)	0.0089(11)	-0.0048(11)
C10	0.0277(13)	0.0389(15)	0.0383(14)	-0.0021(12)	0.0094(11)	-0.0027(11)
C11	0.099(3)	0.061(2)	0.0397(17)	0.0028(16)	0.0310(19)	0.010(2)
C12	0.0432(17)	0.0338(16)	0.077(2)	-0.0130(15)	0.0238(16)	0.0039(13)
C13	0.0345(16)	0.0530(19)	0.083(3)	-0.0080(18)	0.0281(16)	0.0064(14)
C14	0.0310(13)	0.0260(13)	0.0447(15)	0.0099(11)	0.0091(11)	0.0003(10)
C15	0.0323(13)	0.0518(17)	0.0235(12)	0.0015(11)	0.0075(10)	-0.0020(12)
C16	0.0414(16)	0.0291(14)	0.0629(19)	-0.0060(13)	0.0147(14)	0.0038(12)
C17	0.0454(19)	0.049(2)	0.112(3)	-0.013(2)	0.017(2)	0.0209(16)
C18	0.062(2)	0.051(2)	0.060(2)	-0.0201(17)	0.0189(17)	0.0056(16)
C19	0.0392(16)	0.071(2)	0.0392(16)	0.0173(15)	0.0043(13)	-0.0029(15)
C20	0.0401(18)	0.118(4)	0.052(2)	0.036(2)	-0.0039(15)	0.000(2)
C21A	0.072(3)	0.087(4)	0.035(2)	0.008(2)	0.019(2)	-0.031(3)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table 8g. Derived Atomic Coordinates and Displacement Parameters for H-Atoms for **10**.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1	-0.1367	0.1876	0.0757	0.031
H4	-0.0197	-0.0517	0.2657	0.050
H5	-0.2194	-0.0896	0.2217	0.063
H6	-0.3764	-0.0130	0.1427	0.060
H7	-0.3367	0.1046	0.1092	0.047
H11A	-0.1452	0.2039	0.4559	0.077
H11B	-0.0360	0.1642	0.4248	0.077
H11C	-0.1687	0.1316	0.3866	0.077
H12A	-0.1067	0.3373	0.3551	0.060
H12B	-0.0904	0.3414	0.2307	0.060
H12C	0.0115	0.3055	0.3291	0.060
H13A	-0.3440	0.2737	0.2604	0.065
H13B	-0.3606	0.1995	0.1962	0.065
H13C	-0.3292	0.2688	0.1355	0.065
H14A	0.0078	0.2791	0.0869	0.041
H14B	0.1471	0.2954	0.1004	0.041
H14C	0.0979	0.2886	0.2094	0.041
H15A	0.0167	0.1825	-0.0253	0.043
H15B	0.1112	0.1199	0.0158	0.043
H15C	0.1566	0.1955	-0.0134	0.043
H16	0.1957	-0.0567	0.2664	0.053
H17A	0.3761	-0.0858	0.2177	0.083
H17B	0.4035	-0.0413	0.3319	0.083
H17C	0.4084	-0.0037	0.2173	0.083
H18A	0.1905	-0.0751	0.0779	0.069
H18B	0.2049	0.0079	0.0621	0.069
H18C	0.0866	-0.0222	0.0900	0.069
H19A	0.1868	0.0927	0.4597	0.061[a]
H19B	0.2186	-0.0009	0.4267	0.061[b]
H20A	0.3519	0.0419	0.5864	0.088
H20B	0.3898	0.0939	0.4998	0.088
H20C	0.3953	0.0103	0.4837	0.088
H21A	0.1666	-0.0102	0.5461	0.077[a]
H21B	0.1777	-0.0530	0.4377	0.077[a]
H21C	0.0669	-0.0006	0.4289	0.077[a]
H21D	0.1568	0.0575	0.5730	0.107[b]
H21E	0.0642	0.0209	0.4682	0.107[b]
H21F	0.0839	0.1045	0.4695	0.107[b]

[a]Derived with an occupancy factor of 0.7. [b]Derived with an occupancy factor of 0.3.

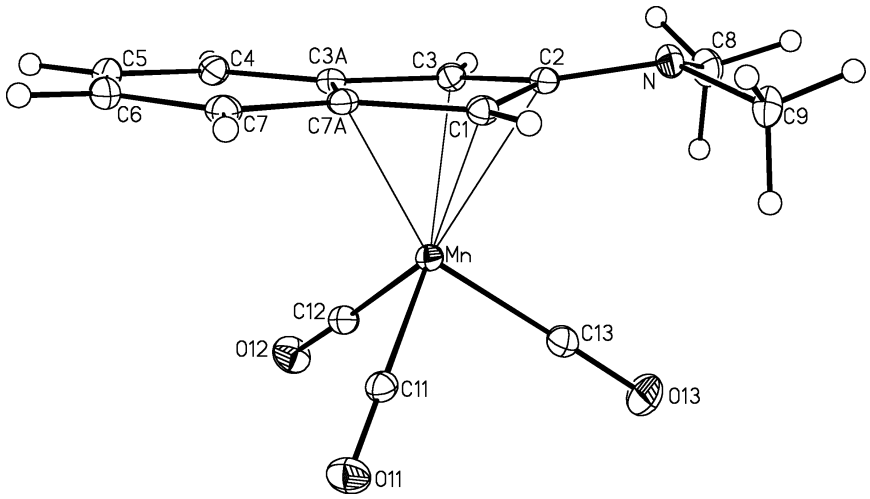

Figure 1h. Perspective view of the η^5–{2-(*N*,*N*-dimethyl)aminoindenyl}tricarbonyl-manganese(I) molecule showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 20% probability level. Hydrogen atoms are shown with arbitrarily small thermal parameters.

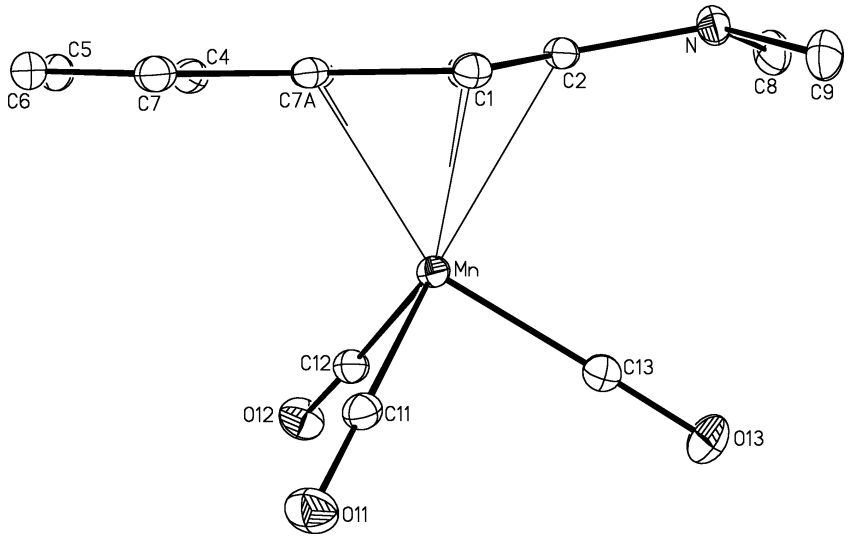

Figure 2h. Alternate view of the molecule showing the slight deviation of C2 from the plane of the indenyl ring system. Hydrogen atoms are not shown.

Table 1h. Crystallographic Experimental Details for **11**.

A. Crystal Data	
formula	$C_{14}H_{12}NO_3Mn$
formula weight	297.19
crystal dimensions (mm)	$0.53 \times 0.26 \times 0.26$
crystal system	triclinic
space group	$P\bar{1}$ (No. 2)
unit cell parameters[a]	
a (Å)	6.9708 (4)
b (Å)	7.1061 (4)
c (Å)	13.3302 (7)
α (deg)	80.2151 (8)
β (deg)	81.6179 (8)
γ (deg)	88.1763 (8)
V (Å^3)	643.74 (6)
Z	2
ρ_{calcd} (g cm^{-3})	1.533
μ (mm^{-1})	1.027
B. Data Collection and Refinement Conditions	
diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.2°) (20 s exposures)
data collection 2θ limit (deg)	52.74
total data collected	4725 ($-8 \le h \le 8$, $-8 \le k \le 8$, $-16 \le l \le 16$)
independent reflections	2605 (R_{int} = 0.0145)
number of observed reflections (*NO*)	2503 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–86*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	Gaussian integration (face-indexed)
range of transmission factors	0.7761–0.6121
data/restraints/parameters	2605 [$F_o^2 \ge -3\sigma(F_o^2)$] / 0 / 174
goodness-of-fit (S)[e]	1.084 [$F_o^2 \ge -3\sigma(F_o^2)$]
final R indices[f]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0241
wR_2 [$F_o^2 \ge -3\sigma(F_o^2)$]	0.0673
largest difference peak and hole	0.321 and –0.237 e Å^{-3}

[a]Obtained from least-squares refinement of 5084 reflections with $5.82° < 2\theta < 52.71°$.

(continued)

Table 1h. Crystallographic Experimental Details for **11**. (continued)

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

[c]Sheldrick, G. M. *Acta Crystallogr*. **1990**, *A46*, 467–473.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted *R*-factors wR_2 and all goodnesses of fit *S* are based on F_o^2; conventional *R*-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. *R*-factors based on F_o^2 are statistically about twice as large as those based on F_o, and *R*-factors based on ALL data will be even larger.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.0336P)^2 + 0.2778P]^{-1}$ where $P = [\mathrm{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2h. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for **11**.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Mn	0.26026(3)	0.31482(3)	0.247365(15)	0.02110(9)*
O11	-0.04507(18)	0.06067(18)	0.36967(10)	0.0393(3)*
O12	-0.02355(19)	0.61017(19)	0.18298(11)	0.0424(3)*
O13	0.2461(2)	0.1329(3)	0.06679(12)	0.0576(4)*
N	0.71286(19)	0.21609(19)	0.15719(10)	0.0274(3)*
C1	0.4978(2)	0.1996(2)	0.32517(11)	0.0235(3)*
C2	0.5858(2)	0.2948(2)	0.22705(11)	0.0232(3)*
C3	0.5156(2)	0.4882(2)	0.21407(11)	0.0242(3)*
C3A	0.4116(2)	0.5199(2)	0.31145(11)	0.0235(3)*
C4	0.3261(2)	0.6871(2)	0.34578(13)	0.0291(3)*
C5	0.2414(2)	0.6727(2)	0.44543(13)	0.0336(4)*
C6	0.2315(2)	0.4959(3)	0.51408(13)	0.0334(4)*
C7	0.3054(2)	0.3317(2)	0.48310(12)	0.0286(3)*
C7A	0.4008(2)	0.3416(2)	0.38027(11)	0.0230(3)*
C8	0.7470(3)	0.3175(3)	0.05171(13)	0.0372(4)*
C9	0.7225(3)	0.0087(2)	0.16738(14)	0.0359(4)*
C11	0.0737(2)	0.1597(2)	0.32198(12)	0.0263(3)*
C12	0.0865(2)	0.4940(2)	0.20694(12)	0.0274(3)*
C13	0.2533(2)	0.2038(3)	0.13761(13)	0.0333(4)*

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$.

Table 3h. Selected Interatomic Distances (Å) for **11**.

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Mn	C1	2.1477(14)	N	C8	1.457(2)
Mn	C2	2.2484(14)	N	C9	1.457(2)
Mn	C3	2.1462(15)	C1	C2	1.427(2)
Mn	C3A	2.1791(14)	C1	C7A	1.442(2)
Mn	C7A	2.1832(14)	C2	C3	1.435(2)
Mn	C11	1.7994(16)	C3	C3A	1.441(2)
Mn	C12	1.7994(16)	C3A	C4	1.427(2)
Mn	C13	1.7837(17)	C3A	C7A	1.430(2)
O11	C11	1.147(2)	C4	C5	1.361(2)
O12	C12	1.146(2)	C5	C6	1.420(3)
O13	C13	1.151(2)	C6	C7	1.364(2)
N	C2	1.3676(19)	C7	C7A	1.425(2)

Table 4h. Selected Interatomic Angles (deg) for **11**.

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C1	Mn	C2	37.80(5)	Mn	C1	C2	74.93(8)
C1	Mn	C3	65.15(5)	Mn	C1	C7A	71.89(8)
C1	Mn	C3A	64.81(5)	C2	C1	C7A	107.91(13)
C1	Mn	C7A	38.87(5)	Mn	C2	N	130.64(10)
C1	Mn	C11	97.92(6)	Mn	C2	C1	67.27(8)
C1	Mn	C12	155.70(6)	Mn	C2	C3	67.13(8)
C1	Mn	C13	109.65(7)	N	C2	C1	126.32(13)
C2	Mn	C3	38.02(5)	N	C2	C3	125.90(13)
C2	Mn	C3A	63.21(5)	C1	C2	C3	107.77(12)
C2	Mn	C7A	63.10(5)	Mn	C3	C2	74.85(8)
C2	Mn	C11	132.44(6)	Mn	C3	C3A	71.78(8)
C2	Mn	C12	135.03(6)	C2	C3	C3A	107.63(12)
C2	Mn	C13	90.99(6)	Mn	C3A	C3	69.32(8)
C3	Mn	C3A	38.91(5)	Mn	C3A	C4	125.11(10)
C3	Mn	C7A	64.83(5)	Mn	C3A	C7A	71.03(8)
C3	Mn	C11	158.56(6)	C3	C3A	C4	132.16(14)
C3	Mn	C12	98.85(6)	C3	C3A	C7A	107.91(12)
C3	Mn	C13	106.38(7)	C4	C3A	C7A	119.93(14)
C3A	Mn	C7A	38.26(5)	C3A	C4	C5	118.38(15)
C3A	Mn	C11	123.23(6)	C4	C5	C6	121.74(15)
C3A	Mn	C12	91.15(6)	C5	C6	C7	121.55(15)
C3A	Mn	C13	145.10(7)	C6	C7	C7A	118.51(15)
C7A	Mn	C11	93.75(6)	Mn	C7A	C1	69.23(8)
C7A	Mn	C12	118.77(6)	Mn	C7A	C3A	70.71(8)
C7A	Mn	C13	148.52(7)	Mn	C7A	C7	125.47(10)
C11	Mn	C12	92.33(7)	C1	C7A	C3A	107.74(13)
C11	Mn	C13	91.36(7)	C1	C7A	C7	132.44(14)
C12	Mn	C13	91.98(7)	C3A	C7A	C7	119.82(14)
C2	N	C8	118.11(13)	Mn	C11	O11	179.88(16)
C2	N	C9	118.26(13)	Mn	C12	O12	178.45(15)
C8	N	C9	114.71(13)	Mn	C13	O13	179.06(16)

Table 5h. Torsional Angles (deg) for **11**.

Atom1	Atom2	Atom3	Atom4	Angle	Atom1	Atom2	Atom3	Atom4	Angle
C2	Mn	C1	C7A	115.03(12)	C12	Mn	C3	C3A	80.76(9)
C3	Mn	C1	C2	-34.97(8)	C13	Mn	C3	C2	-69.72(10)
C3	Mn	C1	C7A	80.07(9)	C13	Mn	C3	C3A	175.48(9)
C3A	Mn	C1	C2	-78.09(9)	C1	Mn	C3A	C3	80.99(9)
C3A	Mn	C1	C7A	36.94(8)	C1	Mn	C3A	C4	-151.31(15)
C7A	Mn	C1	C2	-115.03(12)	C1	Mn	C3A	C7A	-37.53(8)
C11	Mn	C1	C2	158.82(9)	C2	Mn	C3A	C3	38.78(8)
C11	Mn	C1	C7A	-86.15(9)	C2	Mn	C3A	C4	166.49(15)
C12	Mn	C1	C2	-87.12(17)	C2	Mn	C3A	C7A	-79.74(9)
C12	Mn	C1	C7A	27.92(19)	C3	Mn	C3A	C4	127.70(17)
C13	Mn	C1	C2	64.52(10)	C3	Mn	C3A	C7A	-118.52(12)
C13	Mn	C1	C7A	179.55(9)	C7A	Mn	C3A	C3	118.52(12)
C1	Mn	C2	N	119.13(17)	C7A	Mn	C3A	C4	-113.78(16)
C1	Mn	C2	C3	-122.41(12)	C11	Mn	C3A	C3	163.75(9)
C3	Mn	C2	N	-118.46(17)	C11	Mn	C3A	C4	-68.55(15)
C3	Mn	C2	C1	122.41(12)	C11	Mn	C3A	C7A	45.23(11)
C3A	Mn	C2	N	-158.16(15)	C12	Mn	C3A	C3	-102.71(9)
C3A	Mn	C2	C1	82.71(9)	C12	Mn	C3A	C4	24.99(14)
C3A	Mn	C2	C3	-39.69(8)	C12	Mn	C3A	C7A	138.77(9)
C7A	Mn	C2	N	158.75(16)	C13	Mn	C3A	C3	-7.60(15)
C7A	Mn	C2	C1	39.62(8)	C13	Mn	C3A	C4	120.11(15)
C7A	Mn	C2	C3	-82.79(9)	C13	Mn	C3A	C7A	-126.12(13)
C11	Mn	C2	N	90.12(15)	C1	Mn	C7A	C3A	118.55(12)
C11	Mn	C2	C1	-29.01(12)	C1	Mn	C7A	C7	-128.02(17)
C11	Mn	C2	C3	-151.42(10)	C2	Mn	C7A	C1	-38.51(8)
C12	Mn	C2	N	-96.43(15)	C2	Mn	C7A	C3A	80.04(9)
C12	Mn	C2	C1	144.44(10)	C2	Mn	C7A	C7	-166.54(15)
C12	Mn	C2	C3	22.03(13)	C3	Mn	C7A	C1	-80.98(9)
C13	Mn	C2	N	-2.63(15)	C3	Mn	C7A	C3A	37.57(8)
C13	Mn	C2	C1	-121.76(10)	C3	Mn	C7A	C7	150.99(15)
C13	Mn	C2	C3	115.83(10)	C3A	Mn	C7A	C1	-118.55(12)
C1	Mn	C3	C2	34.77(8)	C3A	Mn	C7A	C7	113.42(16)
C1	Mn	C3	C3A	-80.04(9)	C11	Mn	C7A	C1	97.96(9)
C2	Mn	C3	C3A	-114.80(12)	C11	Mn	C7A	C3A	-143.48(9)
C3A	Mn	C3	C2	114.80(12)	C11	Mn	C7A	C7	-30.06(14)
C7A	Mn	C3	C2	77.85(9)	C12	Mn	C7A	C1	-167.30(9)
C7A	Mn	C3	C3A	-36.95(8)	C12	Mn	C7A	C3A	-48.75(10)
C11	Mn	C3	C2	74.97(19)	C12	Mn	C7A	C7	64.67(15)
C11	Mn	C3	C3A	-39.8(2)	C13	Mn	C7A	C1	-0.82(17)
C12	Mn	C3	C2	-164.43(9)	C13	Mn	C7A	C3A	117.74(14)

Table 5h. Torsional Angles for **11**. (continued)

Atom1	Atom2	Atom3	Atom4	Angle
C13	Mn	C7A	C7	-128.84(16)
C1	Mn	C11	O11	18(100)
C2	Mn	C11	O11	36(100)
C3	Mn	C11	O11	-18(100)
C3A	Mn	C11	O11	-47(100)
C7A	Mn	C11	O11	-21(100)
C12	Mn	C11	O11	-140(100)
C13	Mn	C11	O11	128(100)
C1	Mn	C12	O12	-20(6)
C2	Mn	C12	O12	-80(6)
C3	Mn	C12	O12	-66(6)
C3A	Mn	C12	O12	-28(6)
C7A	Mn	C12	O12	0(6)
C11	Mn	C12	O12	95(6)
C13	Mn	C12	O12	-173(6)
C1	Mn	C13	O13	160(11)
C2	Mn	C13	O13	-166(11)
C3	Mn	C13	O13	-131(11)
C3A	Mn	C13	O13	-126(11)
C7A	Mn	C13	O13	161(11)
C11	Mn	C13	O13	62(11)
C12	Mn	C13	O13	-31(11)
C8	N	C2	Mn	73.85(18)
C8	N	C2	C1	163.79(15)
C8	N	C2	C3	-15.5(2)
C9	N	C2	Mn	-71.76(18)
C9	N	C2	C1	18.2(2)
C9	N	C2	C3	-161.13(15)
Mn	C1	C2	N	-124.64(15)
Mn	C1	C2	C3	54.77(10)
C7A	C1	C2	Mn	-64.83(10)
C7A	C1	C2	N	170.53(14)
C7A	C1	C2	C3	-10.06(16)
Mn	C1	C7A	C3A	-60.51(10)
Mn	C1	C7A	C7	119.61(16)
C2	C1	C7A	Mn	66.85(10)
C2	C1	C7A	C3A	6.33(16)
C2	C1	C7A	C7	-173.54(15)
Mn	C2	C3	C3A	64.79(10)
N	C2	C3	Mn	124.56(15)
N	C2	C3	C3A	-170.65(14)
C1	C2	C3	Mn	-54.86(10)
C1	C2	C3	C3A	9.93(16)
Mn	C3	C3A	C4	-119.18(17)
Mn	C3	C3A	C7A	60.84(10)
C2	C3	C3A	Mn	-66.84(10)
C2	C3	C3A	C4	173.98(15)
C2	C3	C3A	C7A	-6.00(16)
Mn	C3A	C4	C5	89.10(17)
C3	C3A	C4	C5	-177.80(15)
C7A	C3A	C4	C5	2.2(2)
Mn	C3A	C7A	C1	59.58(10)
Mn	C3A	C7A	C7	-120.53(13)
C3	C3A	C7A	Mn	-59.76(10)
C3	C3A	C7A	C1	-0.18(16)
C3	C3A	C7A	C7	179.71(13)
C4	C3A	C7A	Mn	120.26(13)
C4	C3A	C7A	C1	179.84(13)
C4	C3A	C7A	C7	-0.3(2)
C3A	C4	C5	C6	-1.9(2)
C4	C5	C6	C7	-0.4(2)
C5	C6	C7	C7A	2.4(2)
C6	C7	C7A	Mn	-88.59(17)
C6	C7	C7A	C1	177.87(15)
C6	C7	C7A	C3A	-2.0(2)

Table 6h. Least-Squares Planes for **11**.

Plane	Coefficients[a]			Defining Atoms with Deviations (Å)[b]			
1	5.856(8)	2.651(9)	7.825(19)	5.988(3)			
				C1	C2	C3	
				N	-0.011(4)		
2	6.423(3)	1.993(6)	6.198(11)	5.611(4)			
				C3	0.0006(5)	C3A	-0.0010(8)
				C7A	0.0010(8)	C1	-0.0006(5)
3	6.4731(16)	1.937(4)	5.985(7)	5.526(3)			
				C3A	0.0088(10)	C4	-0.0148(11)
				C5	0.0057(11)	C6	0.0098(11)
				C7	-0.0152(11)	C7A	0.0057(10)
4	6.286(2)	2.181(5)	6.663(9)	5.779(2)			
				C1	-0.0482(9)	C2	0.0590(9)
				C3	-0.0468(9)	C3A	0.0171(9)
				C7A	0.0189(9)		
				Mn	-1.8083(7)	N	0.221(2)

Dihedral angle between planes 1 and 2: 9.99(17)°

Dihedral angle between planes 2 and 3: 1.11(8)°

Dihedral angle between planes 3 and 4: 3.84(7)°

[a]Coefficients are for the form $ax+by+cz = d$ where x, y and z are crystallographic coordinates.
[b]Underlined atoms were not included in the definition of the plane.

Table 7h. Anisotropic Displacement Parameters (U_{ij}, Å^2) for **11**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mn	0.02041(13)	0.02174(13)	0.02189(13)	-0.00460(9)	-0.00433(8)	-0.00034(8)
O11	0.0344(6)	0.0392(7)	0.0414(7)	-0.0010(5)	-0.0006(5)	-0.0106(5)
O12	0.0367(7)	0.0385(7)	0.0510(8)	-0.0020(6)	-0.0121(6)	0.0105(5)
O13	0.0556(9)	0.0812(11)	0.0480(8)	-0.0405(8)	-0.0127(7)	0.0027(8)
N	0.0260(6)	0.0292(7)	0.0267(6)	-0.0072(5)	-0.0005(5)	0.0033(5)
C1	0.0225(7)	0.0228(7)	0.0257(7)	-0.0031(5)	-0.0059(5)	-0.0001(5)
C2	0.0200(7)	0.0244(7)	0.0265(7)	-0.0056(5)	-0.0055(5)	-0.0006(5)
C3	0.0241(7)	0.0221(7)	0.0258(7)	-0.0029(6)	-0.0025(5)	-0.0020(5)
C3A	0.0200(6)	0.0244(7)	0.0270(7)	-0.0063(6)	-0.0039(5)	-0.0027(5)
C4	0.0270(7)	0.0251(7)	0.0372(8)	-0.0101(6)	-0.0052(6)	-0.0006(6)
C5	0.0274(8)	0.0375(9)	0.0402(9)	-0.0197(7)	-0.0048(7)	0.0023(7)
C6	0.0245(7)	0.0502(10)	0.0281(8)	-0.0155(7)	-0.0016(6)	-0.0023(7)
C7	0.0237(7)	0.0381(8)	0.0241(7)	-0.0038(6)	-0.0046(6)	-0.0051(6)
C7A	0.0196(6)	0.0262(7)	0.0246(7)	-0.0054(6)	-0.0064(5)	-0.0023(5)
C8	0.0375(9)	0.0447(10)	0.0272(8)	-0.0063(7)	0.0026(7)	0.0023(7)
C9	0.0401(9)	0.0306(8)	0.0381(9)	-0.0126(7)	-0.0028(7)	0.0070(7)
C11	0.0255(7)	0.0265(7)	0.0289(8)	-0.0070(6)	-0.0079(6)	0.0012(6)
C12	0.0265(7)	0.0285(7)	0.0272(7)	-0.0041(6)	-0.0044(6)	-0.0020(6)
C13	0.0264(8)	0.0416(9)	0.0345(9)	-0.0123(7)	-0.0063(6)	0.0023(7)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table 8h. Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms for **11**.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H1	0.5167	0.0622	0.3544	0.028
H3	0.5497	0.5882	0.1520	0.029
H4	0.3283	0.8056	0.3002	0.035
H5	0.1876	0.7839	0.4697	0.040
H6	0.1720	0.4919	0.5832	0.040
H7	0.2936	0.2135	0.5290	0.034
H8A	0.7795	0.4507	0.0517	0.045
H8B	0.6297	0.3135	0.0195	0.045
H8C	0.8547	0.2566	0.0129	0.045
H9A	0.7341	-0.0469	0.2387	0.043
H9B	0.8355	-0.0283	0.1218	0.043
H9C	0.6043	-0.0381	0.1484	0.043

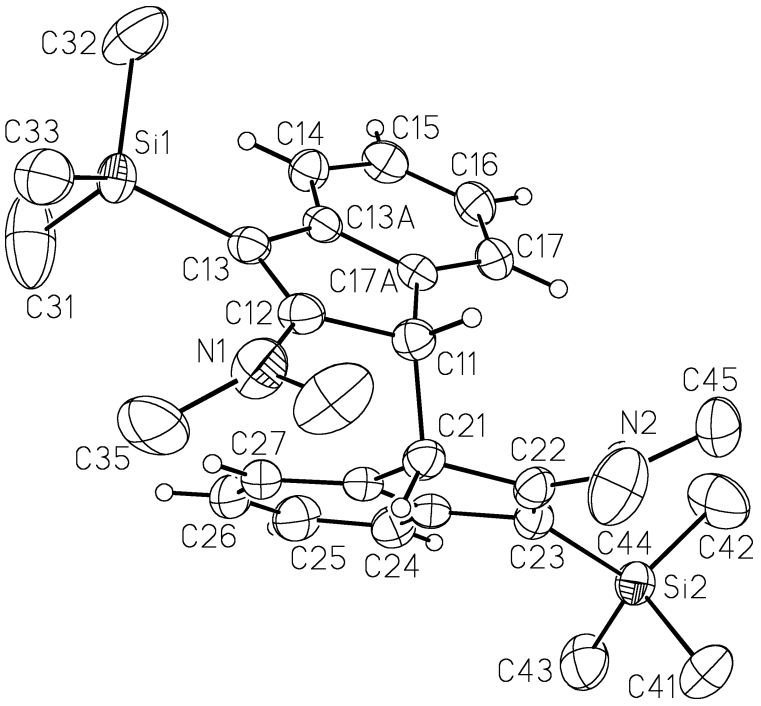

Figure 1i. Perspective view of the *rac*-2,2'-bis(dimethylamino)-3,3'-bis(trimethylsilyl)-1,1'-biindene molecule showing the atom labelling scheme. Non-hydrogen atoms are represented by Gaussian ellipsoids at the 50% probability level. Hydrogen atoms of the indenyl groups are shown with arbitrarily small thermal parameters; methyl hydrogens are not shown.

Table 1i. Crystallographic Experimental Details for *rac*-**12**.

A. Crystal Data	
formula	$C_{28}H_{40}N_2Si_2$
formula weight	460.80
crystal dimensions (mm)	$0.44 \times 0.42 \times 0.14$
crystal system	monoclinic
space group	$P2_1/n$ (an alternate setting of $P2_1/c$ [No. 14])
unit cell parameters[a]	
a (Å)	11.4652 (7)
b (Å)	9.7079 (6)
c (Å)	24.6104 (16)
β (deg)	95.5024 (12)
V (Å^3)	2726.6 (3)
Z	4
ρ_{calcd} (g cm^{-3})	1.123
μ (mm^{-1})	0.148
B. Data Collection and Refinement Conditions	
diffractometer	Bruker PLATFORM/SMART 1000 CCD[b]
radiation (λ [Å])	graphite-monochromated Mo Kα (0.71073)
temperature (°C)	–80
scan type	ω scans (0.3°) (20 s exposures)
data collection 2θ limit (deg)	52.84
total data collected	20951 ($-14 \le h \le 14$, $-12 \le k \le 12$, $-30 \le l \le 30$)
independent reflections	5592 (R_{int} = 0.0451)
number of observed reflections (*NO*)	4130 [$F_o^2 \ge 2\sigma(F_o^2)$]
structure solution method	direct methods (*SHELXS–86*[c])
refinement method	full-matrix least-squares on F^2 (*SHELXL–93*[d])
absorption correction method	multi-scan (*SADABS*)
range of transmission factors	0.9796–0.9379
data/restraints/parameters	5592 [$F_o^2 \ge -3\sigma(F_o^2)$] / 0 / 289
goodness-of-fit (S)[e]	1.043 [$F_o^2 \ge -3\sigma(F_o^2)$]
final R indices[f]	
R_1 [$F_o^2 \ge 2\sigma(F_o^2)$]	0.0617
wR_2 [$F_o^2 \ge -3\sigma(F_o^2)$]	0.1928
largest difference peak and hole	0.469 and –0.427 e Å^{-3}

[a]Obtained from least-squares refinement of 7078 reflections with $4.52° < 2\theta < 51.84°$.

[b]Programs for diffractometer operation, data collection, data reduction and absorption correction were those supplied by Bruker.

(continued)

Table 1i. Crystallographic Experimental Details for *rac*-**12**. (continued)

[c]Sheldrick, G. M. *Acta Crystallogr.* **1990**, *A46*, 467–473.

[d]Sheldrick, G. M. *SHELXL-93*. Program for crystal structure determination. University of Göttingen, Germany, 1993. Refinement on F_o^2 for all reflections (all of these having $F_o^2 \geq -3\sigma(F_o^2)$). Weighted *R*-factors wR_2 and all goodnesses of fit *S* are based on F_o^2; conventional *R*-factors R_1 are based on F_o, with F_o set to zero for negative F_o^2. The observed criterion of $F_o^2 > 2\sigma(F_o^2)$ is used only for calculating R_1, and is not relevant to the choice of reflections for refinement. *R*-factors based on F_o^2 are statistically about twice as large as those based on F_o, and *R*-factors based on ALL data will be even larger.

[e]$S = [\Sigma w(F_o^2 - F_c^2)^2/(n - p)]^{1/2}$ (n = number of data; p = number of parameters varied; $w = [\sigma^2(F_o^2) + (0.1110P)^2 + 1.7503P]^{-1}$ where $P = [\text{Max}(F_o^2, 0) + 2F_c^2]/3$).

[f]$R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^4)]^{1/2}$.

Table 2i. Atomic Coordinates and Equivalent Isotropic Displacement Parameters for *rac*-**12**.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
Si1	0.38062(7)	0.14847(8)	0.08610(3)	0.0325(2)*
Si2	-0.26997(7)	0.59972(9)	0.17171(3)	0.0363(2)*
N1	0.2693(2)	0.4675(3)	0.04669(10)	0.0483(7)*
N2	0.0033(2)	0.7171(2)	0.15531(11)	0.0453(6)*
C11	0.1650(2)	0.4745(3)	0.13220(10)	0.0294(5)*
C12	0.2448(2)	0.4034(3)	0.09469(10)	0.0308(6)*
C13	0.2768(2)	0.2743(3)	0.11212(10)	0.0276(5)*
C13A	0.2191(2)	0.2505(3)	0.16294(10)	0.0270(5)*
C14	0.2173(2)	0.1345(3)	0.19605(11)	0.0318(6)*
C15	0.1593(3)	0.1401(3)	0.24315(11)	0.0362(6)*
C16	0.1033(3)	0.2601(3)	0.25729(11)	0.0360(6)*
C17	0.1032(2)	0.3756(3)	0.22414(10)	0.0321(6)*
C17A	0.1588(2)	0.3689(3)	0.17661(10)	0.0264(5)*
C21	0.0422(2)	0.5059(3)	0.10131(10)	0.0299(6)*
C22	-0.0351(2)	0.5908(3)	0.13588(11)	0.0308(6)*
C23	-0.1360(2)	0.5230(3)	0.14555(10)	0.0305(6)*
C23A	-0.1302(2)	0.3864(3)	0.11958(10)	0.0299(6)*
C24	-0.2056(3)	0.2737(3)	0.11876(12)	0.0379(6)*
C25	-0.1816(3)	0.1570(3)	0.08887(14)	0.0453(7)*
C26	-0.0857(3)	0.1524(3)	0.05910(13)	0.0460(8)*
C27	-0.0102(3)	0.2635(3)	0.05955(12)	0.0380(6)*
C27A	-0.0304(2)	0.3775(3)	0.09052(10)	0.0291(5)*
C31	0.2979(4)	0.0022(5)	0.0526(2)	0.0920(17)*
C32	0.4811(3)	0.0849(4)	0.14490(16)	0.0652(11)*
C33	0.4789(3)	0.2219(4)	0.03756(13)	0.0500(8)*
C34	0.2840(3)	0.6156(4)	0.04438(17)	0.0635(11)*
C35	0.2521(4)	0.3995(5)	-0.00490(14)	0.0712(12)*
C41	-0.2877(3)	0.7784(4)	0.14451(17)	0.0611(10)*
C42	-0.2704(4)	0.5980(5)	0.24722(14)	0.0709(12)*
C43	-0.4066(3)	0.5076(4)	0.14398(16)	0.0588(9)*
C44	0.0765(3)	0.8052(3)	0.12536(18)	0.0615(10)*
C45	-0.0074(3)	0.7623(3)	0.21059(14)	0.0536(8)*

Anisotropically-refined atoms are marked with an asterisk (*). The form of the anisotropic displacement parameter is: $\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$.

Table 3i. Selected Interatomic Distances (Å) for *rac*-**12**.

Atom1	Atom2	Distance	Atom1	Atom2	Distance
Si1	C13	1.862(3)	C13	C13A	1.488(3)
Si1	C31	1.856(4)	C13A	C14	1.391(4)
Si1	C32	1.866(4)	C13A	C17A	1.399(3)
Si1	C33	1.861(3)	C14	C15	1.392(4)
Si2	C23	1.876(3)	C15	C16	1.390(4)
Si2	C41	1.863(4)	C16	C17	1.387(4)
Si2	C42	1.859(4)	C17	C17A	1.386(3)
Si2	C43	1.874(4)	C21	C22	1.527(3)
N1	C12	1.387(3)	C21	C27A	1.508(4)
N1	C34	1.450(4)	C22	C23	1.371(4)
N1	C35	1.428(5)	C23	C23A	1.476(4)
N2	C22	1.373(4)	C23A	C24	1.393(4)
N2	C44	1.449(4)	C23A	C27A	1.409(4)
N2	C45	1.446(4)	C24	C25	1.393(4)
C11	C12	1.527(4)	C25	C26	1.380(5)
C11	C17A	1.505(3)	C26	C27	1.382(4)
C11	C21	1.564(4)	C27	C27A	1.376(4)
C12	C13	1.363(4)			

Table 4i. Selected Interatomic Angles (deg) for *rac*-**12**.

Atom1	Atom2	Atom3	Angle	Atom1	Atom2	Atom3	Angle
C13	Si1	C31	109.80(17)	C13	C13A	C17A	110.1(2)
C13	Si1	C32	108.54(14)	C14	C13A	C17A	119.2(2)
C13	Si1	C33	114.58(14)	C13A	C14	C15	119.4(2)
C31	Si1	C32	110.0(2)	C14	C15	C16	120.7(2)
C31	Si1	C33	108.81(19)	C15	C16	C17	120.3(2)
C32	Si1	C33	104.93(16)	C16	C17	C17A	118.9(2)
C23	Si2	C41	108.13(15)	C11	C17A	C13A	109.1(2)
C23	Si2	C42	114.87(15)	C11	C17A	C17	129.6(2)
C23	Si2	C43	111.65(14)	C13A	C17A	C17	121.3(2)
C41	Si2	C42	110.9(2)	C11	C21	C22	112.2(2)
C41	Si2	C43	104.75(18)	C11	C21	C27A	112.3(2)
C42	Si2	C43	106.10(19)	C22	C21	C27A	101.8(2)
C12	N1	C34	120.8(3)	N2	C22	C21	119.5(2)
C12	N1	C35	121.9(3)	N2	C22	C23	128.0(2)
C34	N1	C35	115.5(3)	C21	C22	C23	112.4(2)
C22	N2	C44	122.2(3)	Si2	C23	C22	126.9(2)
C22	N2	C45	123.1(3)	Si2	C23	C23A	125.3(2)
C44	N2	C45	113.9(3)	C22	C23	C23A	106.4(2)
C12	C11	C17A	101.7(2)	C23	C23A	C24	131.1(2)
C12	C11	C21	111.0(2)	C23	C23A	C27A	110.3(2)
C17A	C11	C21	112.5(2)	C24	C23A	C27A	118.5(2)
N1	C12	C11	119.6(2)	C23A	C24	C25	119.5(3)
N1	C12	C13	127.6(2)	C24	C25	C26	121.0(3)
C11	C12	C13	112.6(2)	C25	C26	C27	120.1(3)
Si1	C13	C12	131.03(19)	C26	C27	C27A	119.6(3)
Si1	C13	C13A	122.48(18)	C21	C27A	C23A	108.7(2)
C12	C13	C13A	106.3(2)	C21	C27A	C27	130.0(2)
C13	C13A	C14	130.7(2)	C23A	C27A	C27	121.2(3)

Table 5i. Torsional Angles (deg) for *rac*-**12**.

Atom1	Atom2	Atom3	Atom4	Angle
C31	Si1	C13	C12	-108.9(3)
C31	Si1	C13	C13A	77.2(3)
C32	Si1	C13	C12	130.7(3)
C32	Si1	C13	C13A	-43.1(3)
C33	Si1	C13	C12	13.8(3)
C33	Si1	C13	C13A	-160.0(2)
C41	Si2	C23	C22	33.8(3)
C41	Si2	C23	C23A	-131.0(2)
C42	Si2	C23	C22	-90.7(3)
C42	Si2	C23	C23A	104.6(3)
C43	Si2	C23	C22	148.5(3)
C43	Si2	C23	C23A	-16.3(3)
C34	N1	C12	C11	36.6(4)
C34	N1	C12	C13	-149.0(3)
C35	N1	C12	C11	-127.2(3)
C35	N1	C12	C13	47.3(5)
C44	N2	C22	C21	32.5(4)
C44	N2	C22	C23	-151.0(3)
C45	N2	C22	C21	-136.1(3)
C45	N2	C22	C23	40.4(5)
C17A	C11	C12	N1	177.8(2)
C17A	C11	C12	C13	2.5(3)
C21	C11	C12	N1	57.8(3)
C21	C11	C12	C13	-117.4(2)
C12	C11	C17A	C13A	-4.4(3)
C12	C11	C17A	C17	176.9(3)
C21	C11	C17A	C13A	114.4(2)
C21	C11	C17A	C17	-64.3(3)
C12	C11	C21	C22	-173.8(2)
C12	C11	C21	C27A	72.2(3)
C17A	C11	C21	C22	72.9(3)
C17A	C11	C21	C27A	-41.0(3)
N1	C12	C13	Si1	10.8(4)
N1	C12	C13	C13A	-174.5(3)
C11	C12	C13	Si1	-174.41(19)
C11	C12	C13	C13A	0.2(3)
Si1	C13	C13A	C14	-8.2(4)
Si1	C13	C13A	C17A	171.97(18)
C12	C13	C13A	C14	176.6(3)
C12	C13	C13A	C17A	-3.2(3)
C13	C13A	C14	C15	177.8(3)
C17A	C13A	C14	C15	-2.4(4)
C13	C13A	C17A	C11	4.9(3)
C13	C13A	C17A	C17	-176.3(2)
C14	C13A	C17A	C11	-174.9(2)
C14	C13A	C17A	C17	3.9(4)
C13A	C14	C15	C16	0.1(4)
C14	C15	C16	C17	0.9(4)
C15	C16	C17	C17A	0.6(4)
C16	C17	C17A	C11	175.6(3)
C16	C17	C17A	C13A	-3.0(4)
C11	C21	C22	N2	58.2(3)
C11	C21	C22	C23	-118.8(2)
C27A	C21	C22	N2	178.5(2)
C27A	C21	C22	C23	1.5(3)
C11	C21	C27A	C23A	115.7(2)
C11	C21	C27A	C27	-62.8(4)
C22	C21	C27A	C23A	-4.5(3)
C22	C21	C27A	C27	177.0(3)
N2	C22	C23	Si2	18.1(4)
N2	C22	C23	C23A	-174.8(3)
C21	C22	C23	Si2	-165.13(19)
C21	C22	C23	C23A	1.9(3)
Si2	C23	C23A	C24	-16.1(4)
Si2	C23	C23A	C27A	162.39(19)
C22	C23	C23A	C24	176.6(3)
C22	C23	C23A	C27A	-5.0(3)
C23	C23A	C24	C25	177.5(3)
C27A	C23A	C24	C25	-0.9(4)
C23	C23A	C27A	C21	6.0(3)
C23	C23A	C27A	C27	-175.3(2)
C24	C23A	C27A	C21	-175.3(2)
C24	C23A	C27A	C27	3.4(4)
C23A	C24	C25	C26	-1.4(5)
C24	C25	C26	C27	1.4(5)
C25	C26	C27	C27A	1.0(5)
C26	C27	C27A	C21	175.0(3)
C26	C27	C27A	C23A	-3.4(4)

Table 6i. Least-Squares Planes for *rac*-**12**.

Plane	Coefficients[a]			Defining Atoms with Deviations (Å)[b]			
1	9.047(6)	3.153(9)	10.910(13)	4.547(3)			
				C12	-0.0274(18)	C13	0.0448(19)
				C13A	0.003(2)	C14	-0.019(2)
				C15	-0.012(2)	C16	0.014(2)
				C17	0.0165(19)	C17A	-0.020(2)
				Si1	0.304(3)	N1	-0.127(4)
				C11	-0.116(3)		
2	5.236(11)	-3.739(6)	18.568(15)	0.092(3)			
				C22	0.0386(18)	C23	-0.056(2)
				C23A	0.002(2)	C24	0.013(2)
				C25	0.021(2)	C26	-0.013(2)
				C27	-0.024(2)	C27A	0.019(2)
				Si2	-0.559(3)	N2	0.128(4)
				C21	0.119(3)		

Dihedral angle between planes 1 and 2: 49.20(8)°

[a]Coefficients are for the form $ax+by+cz = d$ where x, y and z are crystallographic coordinates.
[b]Underlined atoms were not included in the definition of the plane.

Table 7i. Anisotropic Displacement Parameters (U_{ij}, Å^2) for *rac*-**12**.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Si1	0.0336(4)	0.0328(4)	0.0325(4)	-0.0024(3)	0.0113(3)	0.0010(3)
Si2	0.0345(4)	0.0416(5)	0.0335(4)	-0.0031(3)	0.0076(3)	0.0065(3)
N1	0.0596(17)	0.0510(16)	0.0378(14)	0.0167(12)	0.0226(12)	0.0118(13)
N2	0.0518(15)	0.0312(13)	0.0552(16)	-0.0083(11)	0.0178(13)	-0.0074(11)
C11	0.0303(13)	0.0303(13)	0.0278(13)	0.0026(10)	0.0031(10)	0.0002(10)
C12	0.0268(13)	0.0396(15)	0.0263(13)	0.0045(11)	0.0037(10)	0.0011(11)
C13	0.0244(12)	0.0351(14)	0.0232(12)	0.0027(10)	0.0016(9)	0.0006(10)
C13A	0.0251(12)	0.0330(13)	0.0225(12)	-0.0010(10)	0.0004(10)	-0.0012(10)
C14	0.0336(14)	0.0293(13)	0.0328(14)	0.0013(11)	0.0054(11)	0.0010(11)
C15	0.0427(16)	0.0373(15)	0.0287(14)	0.0089(11)	0.0035(12)	-0.0027(12)
C16	0.0426(16)	0.0433(16)	0.0229(12)	0.0012(11)	0.0078(11)	-0.0006(12)
C17	0.0352(14)	0.0369(14)	0.0245(12)	-0.0031(11)	0.0039(10)	0.0021(11)
C17A	0.0259(12)	0.0304(13)	0.0222(12)	0.0000(10)	-0.0007(9)	-0.0030(10)
C21	0.0317(13)	0.0308(13)	0.0277(12)	0.0040(10)	0.0047(10)	0.0046(10)
C22	0.0351(14)	0.0269(13)	0.0306(13)	0.0033(10)	0.0045(11)	0.0048(10)
C23	0.0336(14)	0.0293(13)	0.0290(13)	0.0021(10)	0.0055(10)	0.0032(11)
C23A	0.0327(13)	0.0304(13)	0.0258(12)	0.0046(10)	-0.0010(10)	0.0040(10)
C24	0.0377(15)	0.0356(15)	0.0403(15)	0.0035(12)	0.0039(12)	-0.0001(12)
C25	0.0465(18)	0.0304(15)	0.0570(19)	-0.0014(13)	-0.0048(15)	-0.0037(13)
C26	0.0458(17)	0.0375(16)	0.0520(19)	-0.0140(14)	-0.0091(14)	0.0075(13)
C27	0.0347(14)	0.0431(16)	0.0348(14)	-0.0081(12)	-0.0038(11)	0.0092(12)
C27A	0.0291(13)	0.0323(13)	0.0250(12)	0.0015(10)	-0.0024(10)	0.0057(10)
C31	0.094(3)	0.077(3)	0.114(4)	-0.053(3)	0.054(3)	-0.040(3)
C32	0.059(2)	0.077(3)	0.063(2)	0.033(2)	0.0225(18)	0.034(2)
C33	0.0370(16)	0.071(2)	0.0431(17)	0.0050(16)	0.0116(13)	-0.0007(15)
C34	0.057(2)	0.058(2)	0.081(3)	0.036(2)	0.0307(19)	0.0076(17)
C35	0.079(3)	0.101(3)	0.0334(18)	0.0196(19)	0.0059(17)	0.014(2)
C41	0.060(2)	0.049(2)	0.073(2)	-0.0019(18)	0.0017(19)	0.0214(17)
C42	0.057(2)	0.119(4)	0.0387(19)	-0.003(2)	0.0149(16)	0.006(2)
C43	0.0389(18)	0.068(2)	0.070(2)	-0.0164(19)	0.0099(16)	0.0022(16)
C44	0.067(2)	0.0317(16)	0.089(3)	0.0015(17)	0.027(2)	-0.0060(15)
C45	0.061(2)	0.0409(18)	0.059(2)	-0.0151(15)	0.0029(17)	0.0014(15)

The form of the anisotropic displacement parameter is:

$\exp[-2\pi^2(h^2a^{*2}U_{11} + k^2b^{*2}U_{22} + l^2c^{*2}U_{33} + 2klb^*c^*U_{23} + 2hla^*c^*U_{13} + 2hka^*b^*U_{12})]$

Table 8i. Derived Atomic Coordinates and Displacement Parameters for Hydrogen Atoms for *rac*-**12**.

Atom	*x*	*y*	*z*	U_{eq}, Å^2
H11	0.2021	0.5612	0.1474	0.035
H14	0.2553	0.0522	0.1866	0.038
H15	0.1579	0.0612	0.2659	0.043
H16	0.0649	0.2629	0.2898	0.043
H17	0.0657	0.4581	0.2339	0.039
H21	0.0518	0.5546	0.0662	0.036
H24	-0.2729	0.2765	0.1384	0.045
H25	-0.2320	0.0793	0.0890	0.054
H26	-0.0715	0.0728	0.0383	0.055
H27	0.0553	0.2611	0.0386	0.046
H31A	0.3529	-0.0636	0.0389	0.110
H31B	0.2447	0.0367	0.0220	0.110
H31C	0.2524	-0.0436	0.0790	0.110
H32A	0.5369	0.0193	0.1317	0.078
H32B	0.4352	0.0391	0.1713	0.078
H32C	0.5238	0.1628	0.1625	0.078
H33A	0.5311	0.1496	0.0262	0.060
H33B	0.5258	0.2963	0.0555	0.060
H33C	0.4316	0.2584	0.0055	0.060
H34A	0.3000	0.6425	0.0074	0.076
H34B	0.3497	0.6435	0.0705	0.076
H34C	0.2121	0.6609	0.0536	0.076
H35A	0.2721	0.4624	-0.0337	0.085
H35B	0.1698	0.3716	-0.0119	0.085
H35C	0.3023	0.3178	-0.0045	0.085
H41A	-0.2179	0.8326	0.1566	0.073
H41B	-0.3568	0.8209	0.1581	0.073
H41C	-0.2978	0.7756	0.1045	0.073
H42A	-0.2616	0.5032	0.2606	0.085
H42B	-0.3447	0.6360	0.2572	0.085
H42C	-0.2053	0.6541	0.2637	0.085
H43A	-0.4035	0.4118	0.1566	0.071
H43B	-0.4127	0.5095	0.1040	0.071
H43C	-0.4750	0.5534	0.1568	0.071
H44A	0.0964	0.8887	0.1466	0.074
H44B	0.0341	0.8305	0.0903	0.074
H44C	0.1485	0.7561	0.1189	0.074
H45A	0.0273	0.8542	0.2160	0.064
H45B	0.0337	0.6975	0.2363	0.064
H45C	-0.0904	0.7660	0.2170	0.064