Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

Activation of Boryl-, Borylene and Metalloborylene Complexes by isonitriles

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Experimental Section

General considerations: All syntheses were carried out under argon atmosphere with standard Schlenk and glovebox techniques unless otherwise stated. The complexes [(η^5-C_5Me_5)$(OC)_2$FeBCl_2] (**1**), [(η^5-C_5H_5)$(OC)_2$Mn=B*t*Bu] (**3**) and [{(η^5-C_5Me_5)$(OC)_2$Fe}(μ-B){Cr$(CO)_5$}] (**5**) were prepared according to published procedures.[1-3] Pentane, hexane, benzene and toluene were dried by distillation over Na/K alloy under argon and stored over molecular sieves. C_6D_6 was dried *via* three *freeze-pump-thaw* cycles and stored over molecular sieves. Elemental analyses were obtained from an Elementar Vario MICRO cube instrument. NMR spectra were recorded on a Bruker Avance 400 (^{1}H: 400.1 MHz, ^{11}B: 128.3 MHz, ^{13}C{^{1}H}: 100.6 MHz) and/or a Bruker Avance 500 FT-NMR spectrometer (^{1}H: 500 MHz, ^{11}B: 160 MHz, ^{13}C{^{1}H}: 126 MHz). Chemical shifts are given in ppm, and are referenced against external Me_4Si (^{1}H, ^{13}C{^{1}H}) and $BF_3{\cdot}Et_2O$ (^{11}B).

Preparation of [(η^5-C_5Me_5)$(OC)_2$Fe(CN*t*Bu)(BCl_2)] (2)

tert-Butylisonitrile (78 mg, 0.9 mmol) in 5 mL toluene was added dropwise to a solution of **1** (0.31 g, 0.9 mmol) in 10 mL toluene at –70 °C. After stirring for 30 min at –70 °C the solution was allowed to warm to room temperature and was stirred for a further 60 min. The colour of the solution changed from red to yellow and an insoluble precipitate formed. After filtration and concentration of the solution and storage at –35 °C, a yellow crystalline solid was isolated (271 mg, 71%). Crystals suitable for X-ray diffraction were obtained from a solution of **2** in toluene.

NMR: ^{1}H (C_6D_6, 400.1 MHz): δ = 1.50 (s, 15H, $C_5\mathit{Me}_5$), 1.44 (s, 9H, CN-CNMe_3) ppm. ^{13}C{^{1}H} (C_6D_6, 100.6 MHz): δ = 221.7 (s, *C*N-CNMe_3), 216.7 (s, *C*O), 100.7 (s, C_5Me_5), 61.3 (s, CN-*C*Me_3), 28.5 (s, $C_5\mathit{Me}_5$), 9.7 (s, CNCMe_3) ppm. ^{11}B{^{1}H} (C_6D_6, 128.4 MHz): δ = –6.3 (s, C(*B*Cl_2)N) ppm.
IR (hexane): $\tilde{\nu}$ = 2017 (br, CO), 1969 (br, CO) cm^{-1}.
Elemental analysis (%) found for $FeCl_2ONC_{17}BH_{24}$ C: 49.81 H: 6.06, N: 3.35; calcd. data (%): C: 49.57, H: 5.87; N: 3.40

Reaction of 2 with a Lewis acid
To a solution of **2** (10 mg, 0.024 mmol) in 0.5 mL d_6-benzene was added tris(pentafluoro)phenylborane (12 mg, 0.024 mmol). The color of the solution changed from yellow to orange. The formation of **1** and $(C_6F_5)_3$B-CN*t*Bu can be observed *via* NMR spectroscopy.[4]

NMR: ^{1}H (C_6D_6, 400.1 MHz): δ = 1.42 (s, 15H, $C_5\mathit{Me}_5$), 0.70 (s, 9H, CMe_3) ppm. ^{11}B{^{1}H} (C_6D_6, 128.4 MHz): δ = 95.3 (s, Fe*B*Cl_2), –21.8 (s, $(C_6F_5)_3\mathit{B}$-CNCMe_3) ppm.

Preparation of [(η^5-C_5H_5)$(OC)_2$MnC{N(*t*Bu)B(*t*Bu)(IMe)}] (4)

tert-Butylisonitrile (4.9 mg, 0.059 mmol) was added to a yellow solution of [(η^5-C_5H_5)$(OC)_2$MnB(*t*Bu)(IMe)] (**3**) (20 mg, 0.059 mmol) in benzene (1 mL) at room temperature. After stirring for 5 min, all volatiles were removed under vacuum and the residue washed with pentane (2 × 1 mL) to afford a mixture of **4** as a yellow powder. Yellow single crystals of **4** suitable for X−ray diffraction were obtained by slow evaporation of a benzene solution at room temperature (15.5 mg, 0.037 mmol, 62%).

NMR: ^{1}H (C_6D_6, 400.1 MHz): δ = 5.73 (s, 2H, NC*H*C*H*N), 4.55 (s, 5H, C_5H_5), 3.53 (br, 6H, N-CH_3), 1.59 (s, 9H, N-*t*Bu), 0.89 (s, 9H, *t*Bu); ^{11}B{^{1}H} (C_6D_6, 128.4 MHz) δ = –17.3 (s). ^{1}H (d_8-THF, 400.1 MHz): δ = 7.15 (s, 2H, NC*H*C*H*N), 4.32 (s, 5H, C_5H_5), 4.16 (s, 6H, N-CH_3), 1.57 (s, 9H, N-*t*Bu), 0.68 (s, 9H, *t*Bu); ^{11}B{^{1}H} (d_8-THF, 128.4 MHz) δ = –17.6 (s); ^{13}C{^{1}H} (d_8-THF, 100.6 MHz): δ = 237.9 (s, CO), 234.3 (s, CO), 122.4 (s, N-CH_3), 83.0 (s, C_5H_5), 38.0 (s, N-CH_3), 31.7 (s, C(*C*H_3)$_3$), 30.2 (s, N-C(*C*H_3)$_3$).

IR (hexane) $\tilde{\nu}$ = 1904 (s), 1842 (s) cm^{-1}.

Elemental analysis (%) calcd. for $C_{21}H_{31}BMnN_3O_2$: C 59.59, H 7.38, N 9.93. Found. C 58.90, H 7.50, N 9.53.

Preparation of [(η^5-C_5Me_5)$(OC)_2$Fe(CNCy)(B)$(CNCy)_2$Cr$(CO)_5$] (6)

Cyclohexylisonitrile (110.2 mg, 1.00 mmol) in 5 mL toluene was added dropwise to a solution of **5** (150 mg, 0.333 mmol) in 10 mL toluene at 0 °C. After stirring for 10 min at 0 °C the solution was allowed to warm to room temperature and was stirred for a further hour. The color of the solution changed from maroon to tawny. After removing the solvent *in vacuo*, the dark brown solid residue was extracted with hexane (20 mL). After concentration of the solution and storage at –70 °C, a yellow solid was isolated (42 mg, 24%). Crystals suitable for X-ray diffraction were obtained from a solution of **6** in toluene.

NMR: ^{1}H (C_6D_6, 400.1 MHz): δ = 4.64 (m, 1H, *Cy*), 3.50 (m, 1H, *Cy*), 2.84 (m, 1H, *Cy*), 2.21-1.41 (m, 20H, *Cy*), 1.33 (s, 15H, C_5*Me*$_5$), 1.29-0.84 (m, 10H, *Cy*) ppm. ^{13}C{^{1}H} (C_6D_6, 100.6 MHz): δ = 226.8 (s, *C*O), 220.9 (s, *C*O), 216.5 (s, *C*O), 214.4 (s, *C*O), 100.1 (s, *C*$_5$Me$_5$), 65.7 (s, CN-*Cy*), 65.3 (s, CN-*Cy*), 62.5 (s, CN-*Cy*), 35.2 (s, CN-*Cy*), 34.9 (s, CN-*Cy*), 33.9 (s, CN-*Cy*), 33.8 (s, CN-*Cy*), 32.0 (s, CN-*Cy*), 31.9 (s, CN-*Cy*), 26.4 (s, CN-*Cy*), 25.9 (s, CN-*Cy*), 25.3 (s, CN-*Cy*), 25.3 (s, CN-*Cy*), 25.0 (s, CN-*Cy*), 25.0 (s, CN-*Cy*), 24.9 (s, CN-*Cy*), 24.4 (s, CN-*Cy*), 9.3 (s, C_5*Me*$_5$) ppm. ^{11}B{^{1}H} (C_6D_6, 128.4 MHz): δ = –8.8 (s) ppm.

IR (hexane): $\tilde{\nu}$ = 2048, 2014, 1966, 1928, 1913, 1762 cm^{-1}.

Elemental analysis (%) found for $FeCrO_7N_3C_{38}BH_{48}$**:** C: 59.12 H: 6.25, N: 5.38 Calcd. data: C: 58.70, H: 6.22; N: 5.40.

Crystal structure determination

The crystal data of **2**, **4** and **6** were collected on a Bruker X8-Apex 2 (Apex2 CCD-detector, Nonius FR-591 rotating anode generator) with multi-layer mirror monochromated $Mo_{K\alpha}$ radiation. The structures were solved using the intrinsic phasing method (ShelXT), expanded using Fourier techniques and refined with the ShelXL software package (see CIF files for software versions).[5] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were assigned to idealised geometric positions and included in structure factor calculations. Additional details on refinement can be found in the CIF files (_refine_special_details section). The ShelXL was interfaced with ShelXLe GUI for most of the refinement steps.[6] The pictures of molecules were prepared using Pov-Ray 3.6.2.[7]

Crystal data for **2**: $C_{41}H_{56}B_2Cl_4Fe_2N_2O_4$, M_r = 916.00, yellow block, 0.25×0.21×0.19 mm^3, monoclinic space group $P2_1/c$, a = 9.156(5) Å, b = 10.840(6) Å, c = 22.940(12) Å, β = 100.259(15)°, V = 2240(2) Å^3, Z = 2, ρ_{calcd} = 1.358 g·cm^{-3}, m = 0.927 mm^{-1}, F(000) = 956, T = 100(2) K, R_1 = 0.0265, wR^2 = 0.0592, 4585 independent reflections [2θ≤52.74°] and 290 parameters. CCDC: 1060845.

Crystal data for **4**: $C_{21}H_{31}BMnN_3O_2$, M_r = 423.24, yellow block, 0.43×0.26×0.15 mm^3, monoclinic space group $P2_1/c$, a = 9.5331(4) Å, b = 12.8390(6) Å, c = 18.2760(8) Å, β = 97.4560(10)°, V = 2217.99(17) Å^3, Z = 4, ρ_{calcd} = 1.267 g·cm^{-3}, m = 0.615 mm^{-1}, F(000) = 896, T = 100(2) K, R_1 = 0.0316, wR^2 = 0.0734, 4370 independent reflections [2θ≤52.04°] and 261 parameters. CCDC: 1060846.

Crystal data for **6**: $C_{38}H_{48}BCrFeN_3O_7$, M_r = 777.45, yellow block, 0.80×0.40×0.30 mm^3, monoclinic space group $P2_1$, a = 10.800(3) Å, b = 18.449(6) Å, c = 19.691(6) Å, β = 96.230(9)°, V = 3900(2) Å^3, Z = 4, ρ_{calcd} = 1.324 g·cm^{-3}, m = 0.700 mm^{-1}, F(000) = 1632, T = 100(2) K, R_1 = 0.0241, wR^2 = 0.0575, 16544 independent reflections [2θ≤53.54°] and 929 parameters. CCDC: 1060847.

Crystallographic data have been deposited with the Cambridge Crystallographic Data Center as supplementary publication no. CCDC 1060845 (**2**), 1060846 (**4**) and 1060847 (**6**). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif

Computational Details

All calculations were carried out in the Gaussian 09 software suite.[8] NBO calculations were carried out with NBO 3.1[9] within the Gaussian software. All geometries were energetically minimized at the B3LYP/6-311+G(d,p) level of theory. For each structure in this work frequency analysis indicated no imaginary frequencies, allowing the description of each structure as a minimum on the potential energy surface. All given energies are in kcal/mol and are ZPE corrected.

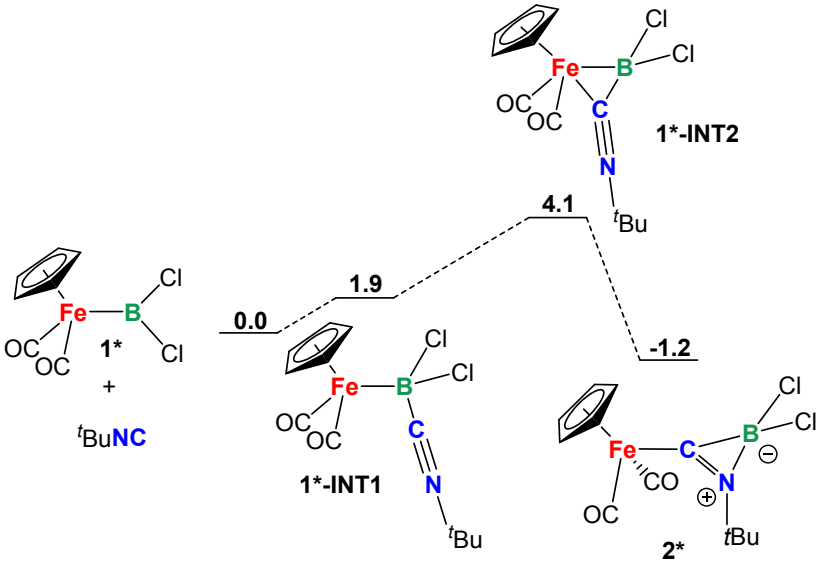

Fig. S1. Reaction pathway for the insertion of *t*BuNC into a model compound of **1** (Cp swapped for Cp*). All points are intermediate geometries (minima with no imaginary frequencies). The relevant transition states were not located. The listed energies are values for $\Delta G_{298.15}$ in kcal/mol. Calculations were carried out at the B3LYP/6-311+G(d,p) level of theory.

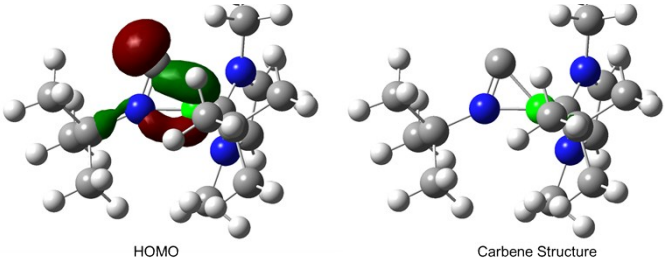

Fig. S2. The structure of the free carbene fragment and a depiction of its HOMO as determined at the B3LYP/6-311+G(d,p) level of theory.

Compound 1*

B	1.33188200	-0.00060500	-0.16428300
O	-0.26968700	-2.13072800	2.17174500
C	-0.39088200	-1.28860000	1.40500100
O	-0.26808800	2.13955200	2.16405100
C	-0.38999600	1.29493800	1.40016600
C	-0.72817300	-0.00319600	-1.92157600

H	0.11071400	-0.00407600	-2.60063300
C	-1.38953700	1.14847000	-1.41130700
H	-1.11984700	2.17393100	-1.61106100
C	-2.48474900	0.70433800	-0.60303300
H	-3.17577800	1.34056600	-0.07112100
C	-2.48401700	-0.70741500	-0.60032300
H	-3.17434900	-1.34229900	-0.06589800
C	-1.38831900	-1.15357700	-1.40679900
H	-1.11746600	-2.17952400	-1.60242700
Fe	-0.61419700	0.00097200	0.21005100
Cl	2.28382600	1.49546700	-0.42999400
Cl	2.28221400	-1.49847800	-0.42576600

Compound 1*_INT1

B	-0.16204900	-1.14837100	-0.32006700
O	-3.45686500	-1.65442600	0.55707200
C	-2.64738700	-0.85063000	0.44965000
O	-0.40210800	0.34967300	2.95970300
C	-0.82502500	0.34891000	1.89051600
C	-0.84705500	1.58225000	-1.47136500
H	-0.08425700	1.25615100	-2.15998900
C	-0.65381800	2.35978700	-0.29883900
H	0.28415700	2.75696200	0.05832100
C	-1.93403300	2.56103200	0.31259600
H	-2.12247100	3.10566700	1.22534800
C	-2.89921500	1.89361800	-0.47158000
H	-3.95730700	1.83986900	-0.26424700
C	-2.22719900	1.27338100	-1.57460600
H	-2.68393600	0.67716400	-2.34866500
Fe	-1.47118900	0.45672900	0.25062900
Cl	-0.06104900	-2.63232000	0.84733700
Cl	-0.41742000	-1.72940800	-2.09530800
C	1.27800700	-0.54441600	-0.25599000
N	2.33236500	-0.07369000	-0.15842100
C	3.69633600	0.40146800	-0.00549400
C	4.37026300	-0.48596700	1.05513600
H	4.37575900	-1.53116300	0.74129000
H	5.40255900	-0.15685900	1.19259200
H	3.85085400	-0.41268900	2.01226900
C	3.64219200	1.86898200	0.44929400
H	4.65984800	2.24267000	0.58108300
H	3.14213100	2.49077300	-0.29616700
H	3.11409300	1.96291700	1.40007800
C	4.38948700	0.26447300	-1.37135300
H	3.88734400	0.87057300	-2.12797800
H	5.42305400	0.60603000	-1.28436800
H	4.39321600	-0.77525500	-1.70311500

Compound 1*_INT2

O	0.64587700	-1.06380900	2.97312400
C	0.90639400	-0.78372200	1.89605200
B	-0.60664300	1.47231200	-0.24154400
O	2.60220900	2.15405300	0.85847200

C	2.01669400	1.20113100	0.61046600
C	1.11404300	-1.36749300	-1.70185400
H	0.24315600	-1.24493500	-2.32520500
C	1.27217900	-2.33673100	-0.67522900
H	0.54502200	-3.08047900	-0.39161300
C	2.55533500	-2.13185400	-0.07779200
H	2.97288100	-2.70273600	0.73805000
C	3.16821500	-1.02940000	-0.71657400
H	4.13553500	-0.61362700	-0.47836400
C	2.26626100	-0.54524900	-1.72070100
H	2.43641700	0.29408300	-2.37708000
C	-0.74053100	-0.00838400	0.01337300
N	-1.51992200	-0.97824700	0.12343000
C	-2.99981700	-0.90550800	-0.05119900
Fe	1.32850300	-0.39599700	0.20833300
Cl	-0.79035400	2.65450400	1.08696800
Cl	-0.32863300	2.12081000	-1.88804000
C	-3.54215200	0.48077200	-0.42298400
H	-3.33661800	1.21762700	0.35624500
H	-3.11917700	0.84148400	-1.36385700
H	-4.62716900	0.42821600	-0.54850800
C	-3.59886400	-1.36876700	1.28811200
H	-3.34560900	-0.66846600	2.08806600
H	-4.68856300	-1.42972400	1.21682000
H	-3.21085600	-2.35256100	1.56054600
C	-3.34223500	-1.91997300	-1.15591000
H	-2.94698500	-2.90698100	-0.90545100
H	-4.42607600	-1.99986000	-1.27732900
H	-2.91539800	-1.61115700	-2.11435300

Compound 2*

C	1.93818000	1.70745500	0.77122300
C	2.81811300	0.76918300	1.36368300
C	3.61792600	0.18464400	0.32927100
C	3.21316900	0.77043700	-0.89676100
C	2.16500700	1.70168900	-0.63169700
H	1.17971800	2.27723000	1.28594100
H	2.87858000	0.53875800	2.41692600
H	4.39013600	-0.55746600	0.46056700
H	3.61824200	0.53827200	-1.87077900
H	1.62979500	2.28897200	-1.36158300
C	1.31627200	-1.63094000	1.09329200
C	1.33352900	-1.22725000	-1.51279400
O	1.20232500	-2.49375100	1.83585100
O	1.23337900	-1.82351200	-2.48249700
C	-0.33409700	0.18732300	-0.02030900
N	-1.55692500	-0.22333900	-0.01026700
B	-1.45450100	1.28578100	-0.01931000
C	-2.41267500	-1.43966400	0.05439700
C	-3.73652700	-1.07791900	-0.63320300
H	-3.57519900	-0.81753400	-1.68137600
H	-4.42299500	-1.92713700	-0.58710900
H	-4.20781000	-0.22465000	-0.14125000
C	-2.64765900	-1.75783900	1.54110000
H	-1.71268800	-2.01859500	2.04203300

H	-3.08520400	-0.89951000	2.05445600
H	-3.33273000	-2.60499900	1.63358900
C	-1.73567200	-2.61158000	-0.66359400
H	-1.54302300	-2.37352800	-1.71178700
H	-0.79568600	-2.89409900	-0.18689300
H	-2.39297300	-3.48415900	-0.63072300
Fe	1.54365600	-0.26859500	-0.02625500
Cl	-1.84337400	2.22128600	1.53268700
Cl	-1.87964200	2.21172800	-1.56006600

Compound 3

Mn	-1.28766400	-0.49131300	0.19250500
B	0.30011300	0.70675900	-0.07351800
O	0.23393900	-2.97603700	0.52980600
C	-0.33639700	-1.96689300	0.39648100
O	-0.92490500	0.37450800	2.97451100
C	-1.04998900	0.02428900	1.86742500
C	-2.41382100	0.37738200	-1.49064200
H	-2.02739700	1.10355900	-2.18844900
C	-3.11287300	0.66123100	-0.29119300
H	-3.33762000	1.63901900	0.10233000
C	-3.47875800	-0.58273200	0.30631500
H	-4.01313200	-0.70397800	1.23632800
C	-3.02394100	-1.62654400	-0.53078900
H	-3.14515200	-2.68430500	-0.35275800
C	-2.35324300	-1.03712600	-1.64421800
H	-1.91231400	-1.57371500	-2.47071100
C	0.47684000	2.32501700	-0.18248700
C	1.46351800	2.82469100	0.90658500
H	1.61575800	3.90625900	0.80418100
H	2.44703200	2.35138800	0.82885000
H	1.07328200	2.65256900	1.91427800
C	1.08434700	2.69536300	-1.55972200
H	0.44003100	2.38375200	-2.38791000
H	2.07338200	2.25073300	-1.70910200
H	1.20600500	3.78289300	-1.63638300
C	-0.82343600	3.13278800	-0.01036900
H	-1.31025000	2.91136300	0.94210900
H	-1.53923900	2.92989200	-0.80844700
H	-0.60646400	4.20831100	-0.03155500
C	1.68508800	-0.10054500	-0.17760800
N	2.51304200	-0.52603900	0.81561500
C	3.51023000	-1.34177200	0.29911000
H	4.25132100	-1.80458100	0.92714700
C	3.31722900	-1.40692000	-1.03592900
H	3.86296100	-1.92801700	-1.80306600
N	2.19663500	-0.64004900	-1.31967600
C	2.30770500	-0.33632600	2.25030500
H	3.27650600	-0.19517000	2.73086000
H	1.80851700	-1.20921600	2.67444300
H	1.69350200	0.53999400	2.42692900
C	1.59503800	-0.52686500	-2.64337300
H	0.52074800	-0.38865300	-2.51970400
H	1.77482200	-1.45222100	-3.19116400
H	2.01350700	0.31377800	-3.19868100

Compound 4

Mn	-2.15660400	-0.34629000	0.08696600
B	1.29844700	0.16300800	0.50811400
O	-1.86713700	-2.14569400	2.38995800
C	-1.94478100	-1.41101700	1.49108000
O	-3.09027900	1.83490300	1.82493100
C	-2.69245700	0.98528600	1.14319400
C	-1.98253400	-0.77151000	-2.08278900
H	-1.06301300	-0.68326300	-2.64158000
C	-2.94341600	0.25685100	-1.89484600
H	-2.90673400	1.25260700	-2.30758800
C	-3.99424400	-0.28127600	-1.09086500
H	-4.87791600	0.24866400	-0.76855300
C	-3.68688100	-1.63155500	-0.80032900
H	-4.29178400	-2.31097300	-0.21938900
C	-2.43397800	-1.93843800	-1.41735800
H	-1.93511800	-2.89516400	-1.39618800
C	-0.27007200	0.28004200	0.12693300
N	0.51168300	1.24823500	-0.24542800
C	0.37761900	2.57102300	-0.92736300
C	1.54322500	3.47528300	-0.50295200
H	1.56366600	3.60528500	0.58054000
H	1.42837300	4.46163700	-0.96022600
H	2.50812200	3.07736500	-0.82092300
C	0.42203100	2.33593800	-2.44760700
H	1.34622200	1.82977300	-2.74013500
H	0.37432100	3.28902700	-2.98271900
H	-0.41954000	1.72044700	-2.76910300
C	-0.94110900	3.24736200	-0.53195800
H	-1.79773300	2.63010900	-0.79333600
H	-1.02931100	4.20627600	-1.05116100
H	-0.97944300	3.43451700	0.54263500
C	1.86954700	0.37482000	2.03549200
C	1.95332600	-0.97726900	2.78046400
H	2.31743200	-0.83217000	3.80555600
H	2.65018100	-1.67128900	2.29482400
H	0.97612000	-1.46228700	2.84716100
C	3.28111600	1.00578800	2.07072400
H	3.29992100	1.99530500	1.60210800
H	4.02618100	0.37690600	1.56877100
H	3.62530100	1.13536000	3.10524900
C	0.91928400	1.28837000	2.83552400
H	-0.08557300	0.86450400	2.90135700
H	0.82518100	2.27877000	2.38149900
H	1.28950300	1.43004600	3.85872200
C	2.17435600	-0.87787200	-0.40235000
N	1.95386300	-2.21383000	-0.51250900
C	2.89370000	-2.80400700	-1.33560700
H	2.88935600	-3.85929000	-1.54716300
C	3.72097900	-1.81899400	-1.75762300
H	4.57456400	-1.84607500	-2.41282800
N	3.27264700	-0.64753100	-1.17325600
C	0.89798000	-2.96766100	0.16751200
H	1.28186400	-3.41030000	1.08686000
H	0.54844400	-3.75496300	-0.50056900
H	0.07898600	-2.29309300	0.39567700

C	3.91381800	0.64367300	-1.39766500
H	3.66849000	1.02368500	-2.39117800
H	4.99473800	0.52790700	-1.30904100
H	3.56901000	1.34206300	-0.64441000

Free carbene [:C(NtBu){B(IMe)tBu}]

C	0.82415400	0.21592500	1.66906700
N	1.33272000	-0.16608800	0.55005700
B	0.03281200	0.56016900	0.26767800
C	-3.22131900	-1.43899600	0.46660000
C	-2.84602000	-1.77106900	-0.79253500
H	-4.08095000	-1.73278400	1.04400300
H	-3.31185200	-2.41317400	-1.52028000
C	-0.90030000	-1.24052100	-2.27957800
H	-1.49051900	-0.86532700	-3.11728100
H	0.00990500	-0.65524000	-2.18979000
H	-0.64551400	-2.28802100	-2.45154100
C	-2.29242000	-0.00108600	2.30770700
H	-1.27357100	0.25480500	2.59821000
H	-2.91691000	0.89373200	2.30397100
H	-2.70836100	-0.73688000	2.99678800
C	-1.27453900	-0.37733400	0.04456500
N	-2.25136200	-0.59006900	0.96525700
N	-1.65398400	-1.11224800	-1.03679000
C	2.55645600	-0.94657700	0.19586900
C	2.15151100	-2.42498100	0.07311700
H	1.74604000	-2.78551700	1.02167200
H	1.38900000	-2.56107200	-0.69923900
H	3.01542900	-3.04142100	-0.19274700
C	3.10892100	-0.42928100	-1.13640500
H	3.99336700	-1.00172800	-1.43060900
H	2.36696800	-0.52002000	-1.93476300
H	3.39318600	0.62235400	-1.05812200
C	3.58380100	-0.77032100	1.31824100
H	4.46101100	-1.39599700	1.13055400
H	3.90496900	0.27167400	1.38770100
H	3.14450900	-1.04364800	2.27913300
C	-0.06681600	2.08547900	-0.33012500
C	-0.17270900	2.15679700	-1.87044600
H	-0.22167500	3.19866200	-2.21593100
H	0.69354400	1.69623200	-2.35795300
H	-1.07531600	1.65882800	-2.24381100
C	1.17306300	2.89457500	0.09928800
H	1.09428600	3.93671700	-0.23749400
H	1.28969900	2.89675900	1.18665700
H	2.09256900	2.48035200	-0.32480100
C	-1.31162400	2.79211800	0.25547300
H	-1.26577600	2.83028800	1.34798000
H	-1.38994300	3.82520800	-0.10876600
H	-2.24272400	2.28484200	-0.02662200

Free IMe

C	-0.67751600	-1.21377000	0.00001500

C	0.67744700	-1.21377600	-0.00003500
H	-1.37783100	-2.03288100	-0.00000400
H	1.37775500	-2.03288000	0.00005600
C	2.44709200	0.57223400	-0.00000600
H	2.97123700	0.21480300	0.89041400
H	2.97114300	0.21504500	-0.89058000
H	2.43850500	1.66006500	0.00014200
C	-2.44704100	0.57228100	-0.00001600
H	-2.43842300	1.66011000	0.00007800
H	-2.97109200	0.21506900	-0.89057500
H	-2.97119100	0.21491000	0.89042400
C	0.00001400	0.97985700	0.00001200
N	1.06385600	0.12178200	0.00000700
N	-1.06386800	0.12176100	0.00002500

[(η^5-C_5H_5)$(OC)_2$Mn(IMe)]

Mn	0.82634700	0.00001200	0.13938100
O	0.91420500	2.09302900	2.20122300
C	0.83912300	1.26494800	1.39097300
O	0.91462900	-2.09389700	2.20030600
C	0.83931700	-1.26549000	1.39041300
C	1.63672500	1.15257200	-1.56437900
H	1.40169600	2.17853100	-1.80319900
C	0.99050300	0.00055000	-2.07945500
H	0.13977400	0.00072400	-2.74497200
C	1.63669600	-1.15175200	-1.56493800
H	1.40181100	-2.17758300	-1.80445800
C	2.69856200	-0.70709900	-0.71572800
H	3.38798100	-1.34077700	-0.17875900
C	2.69858500	0.70748000	-0.71537200
H	3.38807500	1.34086600	-0.17815000
C	-3.34982800	0.67550800	-0.31754300
C	-3.34975300	-0.67570800	-0.31765600
H	-4.15816300	1.37911700	-0.41856800
H	-4.15800600	-1.37938900	-0.41882300
C	-1.64416300	-2.47903200	-0.08975700
H	-1.63349200	-2.82485300	0.94543300
H	-2.35957900	-3.07084000	-0.66219200
H	-0.65138400	-2.60403500	-0.51161400
C	-1.64447700	2.47899100	-0.08940000
H	-1.63479400	2.82490900	0.94577200
H	-0.65130900	2.60400600	-0.51032500
H	-2.35937400	3.07070800	-0.66258200
C	-1.18091200	-0.00000100	-0.05592500
N	-2.03028800	-1.07369900	-0.16591100
N	-2.03040400	1.07362000	-0.16576000

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