Synthesis and reactions of a cyclopentadienyl-amidinate titanium *tert*-butoxyimido compound

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SUPPORTING INFORMATION

Additional experimental details

General methods and instrumentation. All manipulations were carried out using standard Schlenk line or dry-box techniques under an atmosphere of argon or dinitrogen. Solvents were either degassed by sparging with dinitrogen and dried by passing through a column of the appropriate drying agent[1] or refluxed over sodium (toluene), potassium (THF) or Na/K alloy (Et$_2$O) and distilled. Deuterated solvents were dried over sodium (C$_6$D$_6$ and toluene-d_8), potassium (THF-d_8) or CaH$_2$ (C$_6$D$_5$Br) distilled under reduced pressure and stored under argon in Teflon valve ampoules. NMR samples were prepared under dinitrogen in 5 mm Wilmad 507-PP tubes fitted with J. Young Teflon valves. ^{1}H, ^{13}C{^{1}H}, ^{13}C{^{19}F}, ^{11}B, ^{19}F and ^{31}P spectra were recorded on Varian Mercury-VX 300 or Varian Unity Plus 500 spectrometers or on a Bruker AVC 500 spectrometer fitted with a ^{13}C cryoprobe. ^{1}H, ^{13}C{^{1}H} and ^{13}C{^{19}F} spectra are referenced internally to residual protio-solvent (^{1}H) or solvent (^{13}C) resonances, and are reported relative to tetramethylsilane (δ = 0 ppm). ^{19}F, ^{11}B and ^{31}P spectra were referenced externally to CFCl$_3$, Et$_2$O·BF$_3$ or an 85% H$_3$PO$_4$ solution, respectively. Assignments were confirmed as necessary with the use of two dimensional ^{1}H-^{1}H, ^{13}C-^{1}H and ^{13}C-^{19}F NMR correlation experiments. IR spectra were recorded on a Perkin Elmer Paragon 1000 FTIR, Nicolet Magna 560 E.S.P. FTIR or Thermo Scientific Nicolet iS5 FTIR spectrometer and samples prepared in a dry-box using NaCl plates either as a Nujol mull or thin film. Mass spectra were recorded by the mass spectrometry service of Oxford University's Department of Chemistry. Elemental analyses were carried out by Elemental Microanalysis Ltd, Devon or by the Elemental Analysis Service at the London Metropolitan University.

Starting materials. Cp*Ti(N^{t}Bu)Cl(py),[2] Cp*Ti{MeC(N^{i}Pr)$_2$}(N^{t}Bu),[3] ^{t}BuONH$_2$,[4] Li[^{t}BuC(N^{i}Pr$_2$)$_2$],[5] MeCC(4-C$_6$H$_4$CF$_3$),[6] Ar^{F_5}CCH,[7] [Et$_3$NH][BPh$_4$][8] and [PhC(NH^{i}Pr)$_2$]Cl[9] were synthesised according to published procedures. All other reagents were purchased from commerical suppliers and (for liquid reagents) degassed before use, unless specified otherwise. Ar^{F_5}CN, Ar′NCO and PhCCMe were dried

over CaH_2 and distilled before use. $Li[PhC(N^iPr)_2]^{10}$ and $Li[MeC(NTol)_2]^5$ were synthesised using modified published procedures given below.

$Li[PhC(N^iPr)_2]$ (16). To a stirred solution of $^iPrNCN^iPr$ (9.71 mL, 62.7 mmol) in ether (50 mL), cooled to 0 °C, was added PhLi (33.0 mL, 1.9M in $^nBu_2O$, 62.7 mmol) in dropwise aliquots immediately producing a light pink precipitate. After 5 h at RT the volatiles were removed under reduced pressure and hexane (50 mL) added. The mixture was cooled to -80 °C yielding **16** as a light pink crystalline solid which was isolated by filtration and dried *in vacuo*. Yield 11.6 g (88%).

$Li[MeC(NTol)_2]$. To a stirred solution of TolNCNTol (1.33 g, 6.00 mmol) in ether (15 mL), cooled to 0 °C, was added MeLi (3.75 mL, 1.6 M in Et_2O, 6.00 mmol) in dropwise aliquots. A colour change to yellow was observed. After 17 h at RT the volatiles were removed under reduced pressure yielding $Li[MeC(NTol)_2]$ as a yellow solid which was washed with hexane (3 x 10 mL) before being dried *in vacuo*. Yield = 1.07 (73%).

$Cp*Ti\{MeC(N^iPr)_2\}(NO^tBu)$ (15). To a solution of $Cp*Ti\{MeC(N^iPr)_2\}(N^tBu)$ (**10,** 0.932 g, 2.36 mmol) in toluene (10 mL), cooled to -78 °C, was added $^tBuONH_2$ in toluene (1.8 M, 1.70 mL, 3.06 mmol) dropwise over a period of 5 min and the solution slowly warmed to RT. A color change from red to dark green/black was observed. After 3.5 h the volatiles were removed under reduced pressure to afford **15** as a dark green oil, which was dried *in vacuo*. Yield 0.941 g (97%). ^1H NMR (C_6D_6, 299.9 MHz, 293 K): δ 3.72 (2 H, sept., $^3J = 6.3$ Hz NC$\underline{H}$MeMe), 2.16 (15 H, s, C_5Me_5), 1.81 (3 H, s, MeCN$_2$), 1.09 (9 H, s, OCMe$_3$), 1.05 (6 H, d, $^3J = 6.6$ Hz, NCH$\underline{Me}$Me), 1.03 (6 H, d, $^3J = 6.3$ Hz, NCHMe$\underline{Me}$) ppm. $^{13}C\{^1H\}$ NMR (C_6D_6, 75.4 MHz, 293 K): δ 162.1 (Me$\underline{C}$N$_2$), 119.2 ($\underline{C}_5Me_5$), 80.1 (O$\underline{C}$Me$_3$), 49.1 (N$\underline{C}$HMeMe), 26.9 (OC$\underline{Me}_3$), 26.6 (NCH$\underline{Me}$Me), 25.5 (NCHMe$\underline{Me}$), 12.1 ($C_5\underline{Me}_5$), 11.6 ($\underline{Me}$CN$_2$) ppm. IR (NaCl plates, Nujol mull, cm^{-1}): 1485 (s, br), 1468 (s, sh), 1416 (s, sh), 1359 (s), 1338 (s), 1317 (m), 1214 (s), 1173 (s), 1149 (s), 1123 (m), 1017 (m), 848 (m), 810 (m), 794 (m), 752 (w), 705 (m), 634 (w), 552 (w). EI-HRMS found (calcd for $[C_{22}H_{41}N_3OTi]^+$): $m/z = 411.2735$ (411.2729).

$Cp*Ti\{PhC(N^iPr)_2\}(N^tBu)$ (18). To a solution of $Cp*Ti(N^tBu)Cl(py)$ (**17**, 0.500g, 1.36 mmol) in benzene (10 mL) was added a solution of $Li[PhC(N^iPr)_2]$ (**16**, 0.342 g, 1.63 mmol) in benzene (10 mL) and heated to 60 °C. After 18 h the volatiles were removed under reduced pressure to afford **18** as a red, waxy oil which was extracted into pentane (3 x 5 mL). The volatiles were removed under reduced pressure and the resultant dark red oil dried *in vacuo*. Yield 0.608 g (98%). ^1H NMR (C_6D_6, 299.9 MHz, 293 K): δ 7.45 (1 H, m, o_a-C_6H_5), 7.19-7.05 (4 H, m, overlapping o_b-C_6H_5, m-C_6H_5, p-C_6H_5), 3.56 (2 H, sept., $^3J = 6.3$ Hz, NC$\underline{H}$MeMe), 2.22 (15 H, s, C_5Me_5), 1.22 (9 H, s, NCMe$_3$), 1.05 (6 H, d, $^3J = 6.3$ Hz, NCHMe$\underline{Me}$), 0.91 (6 H, d, $^3J = 6.3$ Hz, NCHMe$\underline{Me}$) ppm. $^{13}C\{^1H\}$ NMR (C_6D_6, 75.4 MHz, 293 K): δ 165.8 (Me$\underline{C}$N$_2$), 134.9 (i-C_6H_5), 128.8, 128.6, 128.3, 128.2, (p-C_6H_5, m_a-C_6H_5, m_b-

C$_6$H$_5$, o_b-C$_6$H$_5$), 127.5 (o_a-C$_6$H$_5$), 119.4 (C$_5$Me$_5$), 67.3 (NCMe$_3$), 49.6 (NCHMeMe), 33.0 (NCMe$_3$), 26.8 (NCHMeMe), 25.5 (NCHMeMe), 12.9 (C$_5$Me$_5$) ppm. IR (NaCl plates, Nujol mull, cm^{-1}): 1638 (w), 1602 (w), 1528 (w), 1359 (s), 1338 (s), 1243 (s), 1220 (s), 1168 (s), 1140 (m), 1120 (m), 1073 (m), 1016 (s), 952 (w), 801 (m), 780 (s), 738 (w), 703 (s), 583 (w), 539 (m), 506 (w). EI-HRMS found (calcd for [C$_{27}$H$_{43}$N$_3$Ti]$^+$): m/z = 457.2932 (457.2936).

NMR tube scale synthesis of Cp*Ti{PhC(N^{i}Pr)$_2$}{N(O^{t}Bu)C(Ph)(H)O} (25a_int). To a solution of Cp*Ti{PhC(N^{i}Pr)$_2$}(NO^{t}Bu) (**19**, 10.4 mg, 0.0220 mmol) in toluene-d_8 (0.50 mL) pre-cooled to -78 °C in an NMR tube equipped with a J. Young Teflon valve was added PhC(O)H (2.23 μL, 0.0220 mmol). An immediate color change from dark green to yellow was observed. The solution was allowed to warm to -30 °C at which temperature the ^{1}H NMR spectrum showed quantitative conversion to [Cp*Ti{PhC(N^{i}Pr)$_2$}(μ-O)]$_2$ (**23**) and **25a_int** as a mixture of stereoisomers, **25a_int_H$_{upp}$** and **25a_int_H$_{down}$**.

Major isomer: ^{1}H NMR (toluene-d_8, 299.9 MHz, 243 K): δ 7.84 (2 H, app. d, o-C$_6$H$_5$), 7.22 (1 H, s, PhCH), 6.89 – 7.44 (8 H, m, o-C$_6$H$_5$, m-C$_6$H$_5$, p-C$_6$H$_5$, m-C$_6$H$_5$, p-C$_6$H$_5$), 3.53 (2 H, br. sept., ^3J = 6.6 Hz, NCHMeMe), 2.23 (15 H, s, C$_5$Me$_5$), 1.42 (9 H, s, OCMe$_3$), 1.38 (6 H, br. d, ^3J = 6.6 Hz, NCHMeMe), 1.12 (6 H, br. d, ^3J = 6.3 Hz, NCHMeMe) ppm.

Minor isomer: ^{1}H NMR (toluene-d_8, 299.9 MHz, 243 K): δ 7.95 (1 H, s, PhCH), 7.70 (2 H, app. d, o-C$_6$H$_5$), 6.89 – 7.44 (8 H, m, overlapping o-C$_6$H$_5$, m-C$_6$H$_5$, p-C$_6$H$_5$, m-C$_6$H$_5$, p-C$_6$H$_5$), 3.31 (2 H, br. sept., ^3J = 6.3 Hz, NCHMeMe), 2.17 (15 H, s, C$_5$Me$_5$), 1.42 (9 H, s, OCMe$_3$), 1.22 (6 H, d, ^3J = 6.6 Hz, NCHMeMe), 0.98 (6 H, d, ^3J = 6.3 Hz, NCHMeMe) ppm.

NMR tube scale synthesis of Cp*Ti{PhC(N^{i}Pr)$_2$}{N(O^{t}Bu)C(Ph)(Me)O} (25b_int). To a solution of Cp*Ti{PhC(N^{i}Pr)$_2$}(NO^{t}Bu) (**19**, 11.0 mg, 0.0232 mmol) in toluene-d_8 (0.40 mL) pre-cooled to -78 °C in an NMR tube equipped with a J. Young Teflon valve was added PhC(O)Me (2.71 μL, 0.0232 mmol). The solution was allowed to warm to -10 °C at which temperature the ^{1}H NMR spectrum showed quantitative conversion to [Cp*Ti{PhC(N^{i}Pr)$_2$}(μ-O)]$_2$ (**23**) and **25b_int**. ^{1}H NMR (toluene-d_8, 299.9 MHz, 263 K): δ 6.98 – 7.71 (10 H, m, overlapping 2 x C$_6$H$_5$), 3.50 (2 H, br. sept. ^3J = 6.6 Hz, NCHMeMe), 2.22 (15 H, s, C$_5$Me$_5$), 2.05 (3 H, s, Me) 1.42 (9 H, s, OCMe$_3$), 1.35 (6 H, br. d, ^3J = 6.6 Hz, NCHMeMe), 1.11 (6 H, br. d, ^3J = 6.3 Hz, NCHMeMe) ppm.

Low temperature NMR tube scale reaction of Cp*Ti{PhC(N^{i}Pr)$_2$}(NO^{t}Bu) (19) with PhC(O)H and TolC(O)H (1:1 ratio). To a solution of Cp*Ti{PhC(N^{i}Pr)$_2$}(NO^{t}Bu) (**19**, 10.0 mg, 0.0211 mmol) in toluene-d_8 (0.50 mL) pre-cooled to -50 °C in an NMR tube equipped with a J. Young Teflon valve was added PhC(O)H (2.15 μL, 0.0211 mmol). An immediate color change to orange/yellow was observed. After 15 min at -50 °C TolC(O)H (2.49 μL, 0.0211 mmol) was added. Following a further 10 min at -50 °C the solution was left to warm to room temperature and a subtle color change to

yellow observed. The ^{1}H NMR spectrum recorded after 15 min showed quantitative conversion to [Cp*Ti{PhC(N^{i}Pr)$_2$}(μ-O)]$_2$ (**23**) and PhC(NO^{t}Bu)(H) (**25a**), alongside TolC(O)H.

NMR tube scale synthesis of TolC(NO^{t}Bu)H (25d). To a solution of Cp*Ti{PhC(N^{i}Pr)$_2$}(NO^{t}Bu) (**19**, 40.0 mg, 0.0845 mmol) in toluene-d_8 (0.50 mL) in an NMR tube equipped with a J. Young Teflon valve was added TolC(O)H (9.96 μL, 0.0845 mmol) all at RT. An immediate color change to yellow was observed and ^{1}H NMR spectroscopy showed quantitative conversion to **25d** as a mixture of *anti* and *syn* isomers in the ratio 7:3.

Major isomer (anti): ^{1}H NMR (toluene-d_8, 299.9 MHz, 293 K): δ 7.82 (2 H, d, ^3J = 8.4 Hz, o-C$_6$H$_4$Me), 7.30 (1 H, s, TolC(H)), 6.95 (2 H, d, ^3J = 8.1 Hz, m-C$_6$H$_4$Me), 2.28 (3 H, s, C$_6$H$_4$Me), 1.41 (9 H, s, CMe$_3$) ppm. ^{13}C{^{1}H} NMR (toluene-d_8, 75.4 MHz, 293 K): δ 144.7 (TolC(H)), 139.6 (p-C$_6$H$_4$Me), 131.3 (o-C$_6$H$_4$Me), 129.5 (i-C$_6$H$_4$Me), 129.3 (m-C$_6$H$_4$Me), 78.8 (CMe$_3$), 27.7 (CMe$_3$), 21.3 (C$_6$H$_4$Me) ppm

Minor isomer (syn): ^{1}H NMR (toluene-d_8, 299.9 MHz, 293 K): δ 8.08 (1 H, s, TolC(H)), 7.43 (2 H, d, ^3J = 8.1 Hz, o-C$_6$H$_5$), 6.89 (2 H, d, ^3J = 8.1 Hz, m-C$_6$H$_4$Me), 2.01 (3 H, s, C$_6$H$_4$Me), 1.40 (9 H, s, CMe$_3$) ppm. ^{13}C{^{1}H} NMR (toluene-d_8, 75.4 MHz, 293 K): δ 147.5 (TolC(H)), 139.3 (p-C$_6$H$_4$Me), 131.3 (i-C$_6$H$_4$Me), 129.6 (m-C$_6$H$_4$Me), 127.2 (o-C$_6$H$_4$Me), 79.3 (CMe$_3$), 27.9 (CMe$_3$), 21.3 (C$_6$H$_4$Me) ppm.

Common data: FI-HRMS found (calcd for C$_{12}$H$_{17}$NO): m/z = 191.1308 (191.1310).

NMR tube scale reaction of Cp*Ti{PhC(N^{i}Pr)$_2$}(NO^{t}Bu) (19) with PhC(O)H and TolC(O)H (1:1 ratio). To a solution of Cp*Ti{PhC(N^{i}Pr)$_2$}(NO^{t}Bu) (**19**, 15.0 mg, 0.0317 mmol) in C$_6$D$_6$ (0.30 mL) in an NMR tube equipped with a J. Young Teflon valve was added a pre-mixed solution of TolC(O)H (3.74 μL, 0.0317 mmol) and PhC(O)H (3.22 μL, 0.0317 mmol) in C$_6$D$_6$ (0.30 mL) all at RT. An immediate color change from dark green to yellow was observed. The ^{1}H NMR spectrum recorded after 1 h showed quantitative conversion to PhC(NO^{t}Bu)(H) (**25a**) and TolC(NO^{t}Bu)H (**25d**) in a 1:1 ratio, alongside [Cp*Ti{PhC(N^{i}Pr)$_2$}(μ-O)]$_2$ (**23**).

PhC(NO^{t}Bu)Ph (25c). To a solution of Cp*Ti{PhC(N^{i}Pr)$_2$}(NO^{t}Bu) (**19**, 0.250 g, 0.528 mmol) in benzene (5 mL) was added a solution of PhC(O)Ph (0.962 g, 0.528 mmol) in benzene (5 mL) and heated to 70 °C. After 24 h the volatiles were removed under reduced pressure and the resulting solid sublimed (80-100 °C, 8 x 10^{-2} mbar, 5 h) onto a dry ice/acetone cold finger yielding **25c** a cream solid. Yield 0.125 g (93%). ^{1}H NMR (C$_6$D$_6$, 499.9 MHz, 293 K): δ 7.67 (2 H, m, o_a-C$_6$H$_5$), 7.35 (2 H, m, o_b-C$_6$H$_5$), 7.13 -7.07 (6 H, m, overlapping m_a-C$_6$H$_5$, m_b-C$_6$H$_5$ and p_a-C$_6$H$_5$, p_b-C$_6$H$_5$), 1.33 (9 H, s, NOCMe$_3$) ppm. ^{13}C{^{1}H} NMR (C$_6$D$_6$, 125.7 MHz, 293 K): δ 155.3 (PhC(N)Ph), 138.1 (i-C$_6$H$_5$), 134.5 (i-C$_6$H$_5$), 129.9 (o_b-C$_6$H$_5$), 129.0, 128.5, 128.4, 128.4, 128.2 (p_a-C$_6$H$_5$, p_b-C$_6$H$_5$, m_a-C$_6$H$_5$, o_a-C$_6$H$_5$, m_b-C$_6$H$_5$), 79.3 (NOCMe$_3$), 27.8 (NOCMe$_3$) ppm. IR (NaCl plates, Nujol mull, cm^{-1}): 1665 (w), 1639

(w), 1600 (w), 1493 (m), 1445 (s), 1365 (m), 1359 (m), 1325(w), 1276 (m), 1263 (m), 1240 (w), 1193 (m), 1167 (w), 1074 (w), 1039 (w), 1001 (w), 990 (w), 959 (s), 917 (m), 867 (w), 807 (w), 785 (w), 769 (m), 763 (m), 696 (s), 667 (w), 642 (w), 603 (w). ESI$^+$-HRMS found (calcd for [$C_{17}H_{19}NNaO$, M+Na]$^+$): m/z = 276.1354 (276.1359).

Cp*Ti{PhC(N^{i}Pr)$_2$}{NC(Ar^{F2})NO^{t}Bu} (27). To a solution of Cp*Ti{PhC(N^{i}Pr)$_2$}(NO^{t}Bu) (**19**, 0.300 g, 0.634 mmol) in Et$_2$O (5 mL) was added a solution of Ar^{F2}CN (0.881 g, 0.634 mmol) in Et$_2$O (5 mL) all at RT. An immediate color change from green to lime green was observed. After 2 h the volatiles were removed under reduced pressure to afford **27** as a green oil which was dried *in vacuo*. Yield 0.375 g (97%). ^{1}H NMR (C$_6$D$_6$, 499.9 MHz, 293 K): δ 7.49 (1 H, d, ^3J = 7.5 Hz, o_a-C$_6$H$_5$), 7.17 (1 H, m, m_a-C$_6$H$_5$), 7.09 (1 H, t, ^3J = 7.5 Hz, m_b-C$_6$H$_5$), 7.04 (1 H, m, p-C$_6$H$_5$), 6.98 (1 H, d, ^3J = 7.5 Hz, o_b-C$_6$H$_5$), 6.58 (3 H, m, overlapping m-C$_6$F$_2$H$_3$ and p-C$_6$F$_2$H$_3$), 3.47 (2 H, sept., ^3J = 6.0 Hz, NCHMeMe), 2.27 (15 H, s, C$_5$Me$_5$), 1.42 (9 H, s, NOCMe$_3$), 0.88 (6 H, d, ^3J = 6.5 Hz, NCHMeMe), 0.86 (6 H, d, ^3J = 6.0 Hz, NCHMeMe) ppm. ^{13}C{^{1}H} NMR (C$_6$D$_6$, 125.7 MHz, 293 K): δ 166.9 (PhCN$_2$), 159.7 (dd, $^1J_{C-F}$ = 246.0 Hz, $^3J_{C-F}$ = 9.4 Hz, o-C$_6$F$_2$H$_3$), 153.8 (NC(C$_6$F$_2$H$_3$)N), 133.7 (i-C$_6$F$_2$H$_3$), 128.8 (m_a-C$_6$H$_5$), 128.8 (m_b-C$_6$H$_5$), 128.7 (p-C$_6$H$_5$), 128.4 (p-C$_6$F$_2$H$_3$), 127.6 (o_a-C$_6$H$_5$), 127.4 (o_b-C$_6$H$_5$), 123.1 (C$_5$Me$_5$), 115.8 (t, $^2J_{C-F}$ = 23.9 Hz, i-C$_6$F$_2$H$_3$), 110.9 (dd, $^2J_{C-F}$ = 20.4 Hz, $^4J_{C-F}$ = 5.3 Jz m-C$_6$F$_2$H$_3$), 77.3 (NOCMe$_3$), 50.9 (NCHMeMe), 28.0 (NOCMe$_3$), 26.6 (NCHMeMe), 24.4 (NCHMeMe), 12.5 (C$_5$Me$_5$) ppm. ^{19}F{^{1}H} NMR (C$_6$D$_6$, 282.1 MHz, 293 K): δ -112.1 (2 F, m, o-C$_6$F$_2$H$_3$) ppm. IR (NaCl plates, Nujol mull, cm^{-1}): 1622 (m), 1586 (m), 1528 (m), 1430 (br, s), 1361 (s), 1346 (s), 1270 (w), 1259 (m), 1231 (m), 1217 (m), 1195 (m), 1180 (m), 1168 (m), 1160 (m), 1139 (m), 1075 (w), 1060 (w), 1032 (w), 1015 (m), 1003 (s), 955 (m), 939 (m), 915 (w), 777 (m), 746 (w), 739 (w), 705 (m), 678 (w), 654 (w), 571 (w). EI-MS: m/z = 612 [M]$^+$ (65%). Anal. found (calcd. for C$_{34}$H$_{46}$F$_2$N$_4$OTi): C, 66.80 (66.66); H, 7.68 (7.57); N, 9.03 (9.15)%.

NMR tube scale synthesis of Cp*Ti{PhC(N^{i}Pr)$_2$}{NC(Ph)NO^{t}Bu} (28). To Cp*Ti{PhC(N^{i}Pr)$_2$}(NO^{t}Bu) (**19**, 18.8 mg, 0.0397 mmol) in C$_6$D$_6$ (0.50 mL) in an NMR tube equipped with a J. Young Teflon valve was added PhCN (4.05 μL, 0.0397 mmol) all at RT. A color change from green to dark green was observed. After 19 h ^{1}H NMR spectroscopy showed effectively quantitative conversion to **28**. ^{1}H NMR (C$_6$D$_6$, 499.9 MHz, 293 K): δ 7.90 (2 H, dd, ^3J = 8.0 Hz, o-C$_6$H$_5$ of nitrile), 7.23 (2 H, app. t, ^3J = 8.0 Hz, m-C$_6$H$_5$ of nitrile), 7.20 (1 H, app. d, o_a-C$_6$H$_5$), 7.12-7.00 (5 H, m, overlapping o_b-C$_6$H$_5$, m-C$_6$H$_5$, p-C$_6$H$_5$ and p-C$_6$H$_5$ of nitrile), 3.49 (2 H, sept., ^3J = 6.5 Hz, NCHMeMe), 2.24 (15 H, s, C$_5$Me$_5$), 1.45 (9 H, s, NOCMe$_3$), 0.99 (6 H, d, ^3J = 6.5 Hz, NCHMeMe), 0.87 (6 H, d, ^3J = 6.5 Hz, NCHMeMe) ppm. ^{13}C{^{1}H} NMR (C$_6$D$_6$, 125.7 MHz, 293 K): δ 166.6 (PhCN$_2$), 162.7 (NC(C$_6$H$_5$)N), 136.4 (i-C$_6$H$_5$ of nitrile), 133.6 (i-C$_6$H$_5$), 129.5 (o-C$_6$H$_5$ of nitrile), 128.8, 128.8, 128.7, 127.7, 127.7, 127.4 (o_a-C$_6$H$_5$, o_b-C$_6$H$_5$, m-C$_6$H$_5$, p-C$_6$H$_5$, m-C$_6$H$_5$ of nitrile,

p-C$_6$H$_5$ of nitrile), 122.4 (C$_5$Me$_5$), 77.0 (NOCMe$_3$), 50.6 (NCHMeMe), 28.2 (NOCMe$_3$), 26.6 (NCHMeMe), 25.0 (NCHMeMe), 12.4 (C$_5$Me$_5$) ppm.

NMR tube scale reaction of Cp*Ti{PhC(N^{i}Pr)$_2$}{NC(Ar^{F2})NO^{t}Bu} (27) with Ar^{F5}CN. To a solution of Cp*Ti{PhC(N^{i}Pr)$_2$}{NC(Ar^{F2})NO^{t}Bu} (27, 12.9 mg, 0.0211 mmol) in C$_6$D$_6$ (0.50 mL) in an NMR tube equipped with a J. Young Teflon valve was added Ar^{F5}CN (2.66 μL, 0.0211 mmol) all at RT. After 5 min ^{1}H and ^{19}F NMR spectra showed quantitative conversion to Cp*Ti{PhC(N^{i}Pr)$_2$}{NC(Ar^{F5})NO^{t}Bu} (26) and Ar^{F2}CN.

NMR tube scale reaction of Cp*Ti{PhC(N^{i}Pr)$_2$}{NC(Ph)NO^{t}Bu} (28) with Ar^{F5}CN. To a solution of Cp*Ti{PhC(N^{i}Pr)$_2$}{NC(Ph)NO^{t}Bu} (28, 15.0 mg, 0.0260 mmol) in C$_6$D$_6$ (0.50 mL) in an NMR tube equipped with a J. Young Teflon valve was added Ar^{F5}CN (3.27 μL, 0.0260 mmol) all at RT. After 5 min ^{1}H and ^{19}F NMR spectra showed quantitative conversion to Cp*Ti{PhC(N^{i}Pr)$_2$}{NC(Ar^{F5})NO^{t}Bu} (26) and PhCN.

NMR tube scale reaction of Cp*Ti{PhC(N^{i}Pr)$_2$}{N(C(Ar^{F5})NO^{t}Bu)C(Ar^{F5})NC(Ar^{F5})N} (29). A solution of Cp*Ti{PhC(N^{i}Pr)$_2$}{N(C(Ar^{F5})NO^{t}Bu)C(Ar^{F5})NC(Ar^{F5})N} (29) (15.0 mg, 0.0142 mmol) in C$_6$D$_6$ (0.60 mL) was monitored over time. After 23 h, ^{1}H NMR spectroscopy showed a mixture of Cp*Ti{PhC(N^{i}Pr)$_2$}{NC(Ar^{F5})NO^{t}Bu} (26) and Cp*Ti{PhC(N^{i}Pr)$_2$}-{NC(Ar^{F5})NC(Ar^{F5})N(C{Ar^{F5}}NO^{t}Bu)} (29) in a 50:50 ratio.

NMR tube scale synthesis of [PhC(N^{i}PrH)$_2$][BPh$_4$] (33-BPh$_4$). To a solution of Cp*Ti{PhC(N^{i}Pr)$_2$}(NO^{t}Bu) (19, 10.0 mg, 0.0211 mmol) in THF-d_8 (0.25 mL) in an NMR tube equipped with a J. Young Teflon valve was added a solution of [Et$_3$NH][BPh$_4$] (17.8 mg, 0.0422 mmol) in THF-d_8 (0.25 mL) all at RT. An immediate color change to brown was observed and ^{1}H NMR spectroscopy showed quantitative conversion to 33-BPh$_4$. Diffraction-quality crystals were grown from a saturated bromobenzene solution at RT.

Alternative synthesis [PhC(N^{i}PrH)$_2$][BPh$_4$] (33-BPh$_4$). To a solution of Na[BPh$_4$] (0.573 g, 1.67 mmol) in CH$_2$Cl$_2$ (15 mL) was added a solution of [PhC(N^{i}PrH)$_2$]Cl (0.403 g, 1.67 mmol) in CH$_2$Cl$_2$ (10 mL) all at RT. After 48 h the solution was filtered and the volatiles removed under reduced pressure leaving behind a white solid which was extracted into CH$_2$Cl$_2$ (2 x 5 mL). The volatiles were removed under reduced pressure to afford 33-BPh$_4$ as a white solid which was dried *in vacuo*. Yield 0.556 g (63%). An analytically pure sample was obtained by washing with CHCl$_3$ (2 x 5 mL) at RT and by cooling the filtrate to -30 °C yielding a white crystalline solid which was isolated by filtration and dried *in vacuo*. Yield 0.193 g (23%). ^{1}H NMR (THF-d_8, 299.9 MHz, 248 K): δ 8.95 (1 H, br. d, N$_a$^{i}Pr(H)), 8.28 (1 H, br. d, N$_b$^{i}Pr(H)), 7.60-7.55 (1 H, m, *p*-C$_6$H$_5$), 7.51-7.39 (4 H, m, overlapping *o*-C$_6$H$_5$ and *m*-C$_6$H$_5$), 7.27 (8 H, br m, *o*-B(C$_6$H$_5$)$_4$), 6.86 (8 H, t, ^3J = 7.2 Hz, *m*-B(C$_6$H$_5$)$_4$), 6.73 (4 H, t, ^3J = 7.2 Hz, *p*-B(C$_6$H$_5$)$_4$), 3.86 (1 H, br. m, N$_a$(CHMe$_2$)(H)), 3.50 (1 H, br. m, N$_b$(CHMe$_2$)(H)), 1.27 (6

H, d, ^3J = 6.3 Hz, N_a(CH$\underline{Me}_2$)(H)), 1.16 (6 H, d, ^3J = 6.6 Hz, N_b(CH$\underline{Me}_2$)(H)) ppm. ^{13}C{^{1}H} NMR (THF-d_8, 75.4 MHz, 248 K): δ 165.0 (q, $^1J_{BC}$ = 49.3 Hz, i-B(C$_6$H$_5$)$_4$), 163.4 (Ph$\underline{C}$N$_2$), 137.2 (o-B(C$_6$H$_5$)$_4$), 133.2 (i-C$_6$H$_5$), 130.5 (o-C$_6$H$_5$), 129.8 (p-C$_6$H$_5$), 128.3 (m-C$_6$H$_5$), 125.7 (q, $^3J_{BC}$ 2.7 Hz, m-B(C$_6$H$_5$)$_4$), 121.9 (p-B(C$_6$H$_5$)$_4$), 50.1 (N$_b$($\underline{C}$HMe$_2$)(H)), 46.1 (N$_a$($\underline{C}$HMe$_2$)(H)), 23.0 (N$_b$(CH$\underline{Me}_2$)(H)), 21.6 (N$_a$(CH$\underline{Me}_2$)(H)) ppm. ^{11}B{^{1}H} NMR (THF-d_8, 96.2 MHz, 248 K): δ -5 (BPh$_4$) ppm. IR (NaCl plates, Nujol mull, cm^{-1}): 3277 (s), 3226 (m), 3049 (m), 1626 (s), 1577 (m), 1551 (w), 1478 (m), 1426 (m), 1305 (m), 1263 (w), 1171 (w), 1143 (m), 1130 (m), 1066 (w), 1033 (m), 847 (w), 782 (m), 744 (m), 732 (s), 706 (s), 665 (w), 625 (w), 612 (m), 607 (m). FI$^+$-MS: m/z = 204 [PhC(N^{i}HPr)(N^{i}Pr)]$^+$ (100%), [BPh$_3$]$^+$ (82%). Anal. found (calcd. for C$_{37}$H$_{41}$BN$_2$): C, 84.60 (84.72); H, 7.72 (7.88); N, 5.39 (5.34)%.

NMR tube scale synthesis of [Cp*Ti(NO^{t}Bu)(THF-d_8)$_2$][BPh$_4$] (34-BPh$_4$). To a solution of Cp*Ti{PhC(N^{i}Pr)$_2$}(NO^{t}Bu) (**19**, 10.0 mg, 0.0211 mmol) in THF-d_8 (0.25 mL) in an NMR tube equipped with a J. Young Teflon valve was added a solution of [Et$_3$NH][BPh$_4$] (17.8 mg, 0.0422 mmol) in THF-d_8 (0.25 mL). An immediate color change to brown was observed and ^{1}H NMR spectroscopy showed quantitative conversion to **34-BPh$_4$**. ^{1}H NMR (THF-d_8, 299.9 MHz, 248 K): δ 8 7.27 (8 H, br m, o-B(C$_6$H$_5$)$_4$), 6.87 (8 H, t, ^3J = 7.2 Hz, m-B(C$_6$H$_5$)$_4$), 6.74 (4 H, t, ^3J = 7.2 Hz, p-B(C$_6$H$_5$)$_4$), 1.95 (15 H, s, C$_5$Me$_5$), 0.98 (9 H, s, OCMe$_3$) ppm. ^{13}C{^{1}H} NMR (THF-d_8, 75.4 MHz, 248 K): δ 165.0 (1 B, q, $^1J_{BC}$ = 49.3 Hz, i-B(C$_6$H$_5$)$_4$), 137.1 (o-B(C$_6$H$_5$)$_4$) , 125.9 (m-B(C$_6$H$_5$)$_4$), 122.0 (p-B(C$_6$H$_5$)$_4$), 121.8 ($\underline{C}_5$Me$_5$), 83.7 (O$\underline{C}$Me$_3$), 26.4 (OC$\underline{Me}_3$), 10.9 (C$_5$$\underline{Me}_5$) ppm. ^{11}B{^{1}H} NMR (THF-d_8, 96.2 MHz, 248 K): δ -7 (BPh$_4$) ppm. ES$^+$-MS: m/z = 415 [Cp*Ti(NO^{t}Bu)(THF)$_2$]$^+$ (83%), 343 [Cp*Ti(NO^{t}Bu)(THF)]$^+$ (45%). Note that since these ES$^+$-MS samples were prepared in non-deuterated THF, only cations containing C$_4$H$_8$O (as opposed to C$_4$D$_8$O) are observed.

Crystal structure determinations. Crystal data collection and processing parameters for Cp*Ti{PhC(N^{i}Pr)$_2$}(NO^{t}Bu) (**19**), Cp*Ti{PhC(N^{i}Pr)$_2$}{OC(NTol)N(Tol)C(NO^{t}Bu)O} (**22**), PhC(NO^{t}Bu)Ph (**25c**), [Cp*Ti{PhC(N^{i}Pr)$_2$}(μ-O)]$_2$ (**23**), Cp*Ti{PhC(N^{i}Pr)$_2$}{NC(Ar^{F5})NO^{t}Bu} (**26**), Cp*Ti{PhC(N^{i}Pr)$_2$}{NC(Ar^{F5})NC(Ar^{F5})N(C{Ar^{F5}}NO^{t}Bu)} (**29**), [PhC(N^{i}PrH)$_2$][BPh$_4$] (**33-BPh$_4$**) and Cp*Ti{PhC(N^{i}Pr)$_2$}{η^2-ON(H)B(Ar^{F5})$_3$} (**36**) are given in Table S4. Crystals were mounted on glass fibers using perfluoropolyether oil and cooled rapidly in a stream of cold N$_2$ using an Oxford Cryosystems Cryostream unit. Diffraction data were measured using either an Enraf-Nonius KappaCCD or Agilent Technologies Supernova diffractometer using Mo-K_α or Cu-K_α radiation, respectively. As appropriate, absorption and decay corrections were applied to the data and equivalent reflections merged.[11] The structures were solved with SIR92[12] or Superflip,[13] and further refinements and all other crystallographic calculations were performed using the CRYSTALS program suite.[14] Other details of the structure solution and refinements are given in the CIFs. A full listing of atomic

coordinates, bond lengths and angles and displacement parameters for all the structures have been deposited at the Cambridge Crystallographic Data Centre. See Notice to Authors, Issue No. 1.

1Q_Me

HOMO-1 = -5.47eV   HOMO = -5.28eV   HOMO-2 = -5.93eV

1Q_Ph

HOMO = -4.98eV   HOMO-1 = -5.58eV   HOMO-2 = -6.28eV
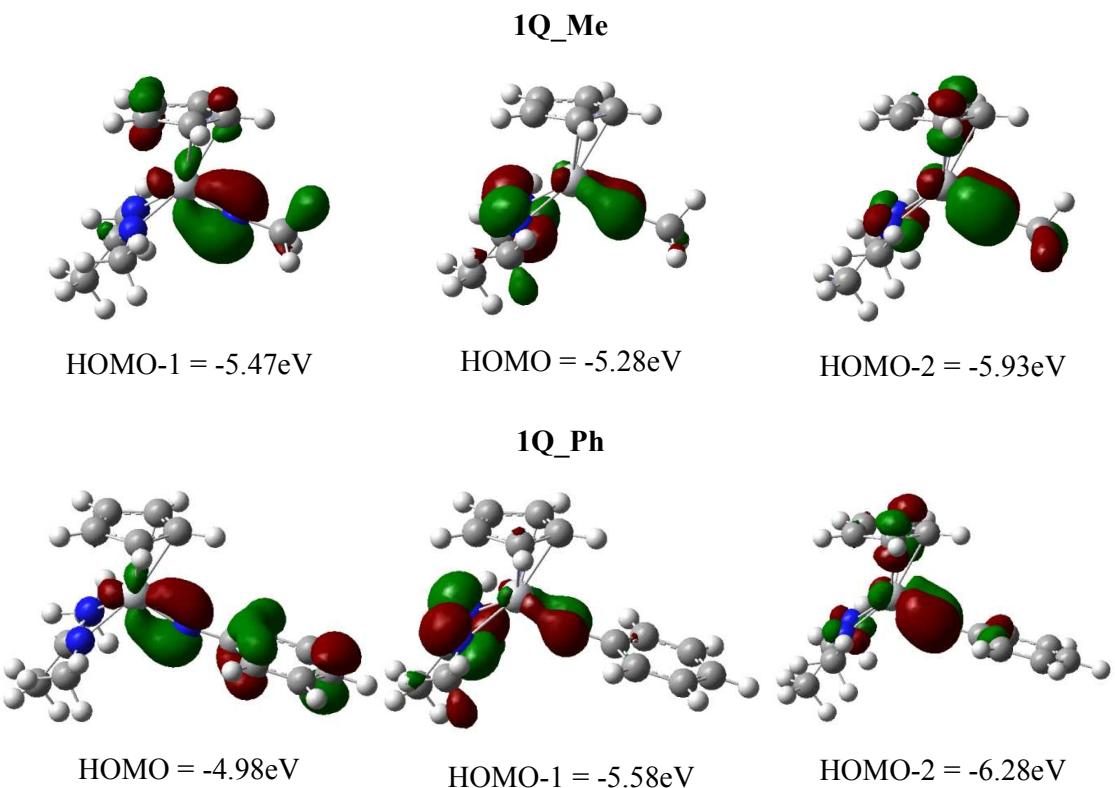
Figure S1. (a) Model compounds CpTi{MeC(NMe)$_2$}(NR) (R = Me (**1Q_Me**) and Ph (**1Q _Ph**)) studied by DFT previously.[15] Associated isosurfaces and energies of the HOMO, HOMO-1 and HOMO-2.

1Q_NMe₂
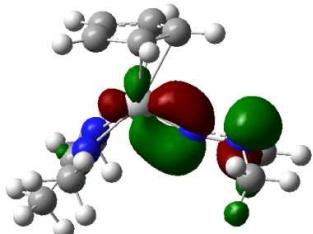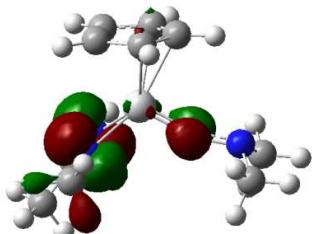
HOMO = -4.30eV   HOMO-1 = -5.25eV   HOMO-2 = -6.09eV
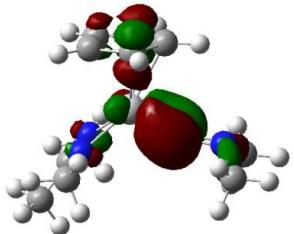
1Q_NPh₂
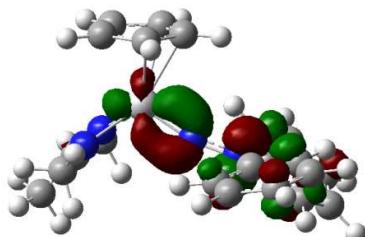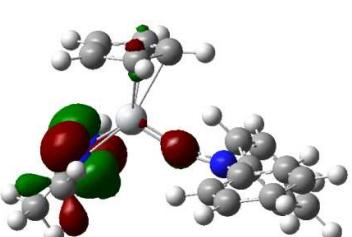
HOMO = -4.24eV   HOMO-1 = -5.50eV   Combination of orbitals

1Q_OMe
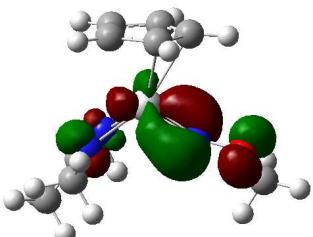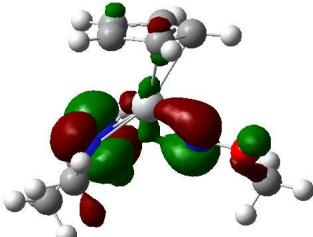
HOMO = -4.92eV   HOMO-1 = -5.39eV   HOMO-2 = -5.93eV
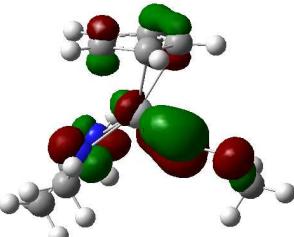
Figure S1. (b) Model compounds CpTi{MeC(NMe)₂}(NR) (R = NMe₂ (**1Q_NMe₂**), NPh₂ (**1Q_NPh₂**) or OMe (**1Q_OMe**)) studied by DFT. Associated isosurfaces and energies of the HOMO, HOMO-1 and HOMO-2. The models **1Q_NMe₂** and **1Q_NPh₂** have been reported previously.[15]
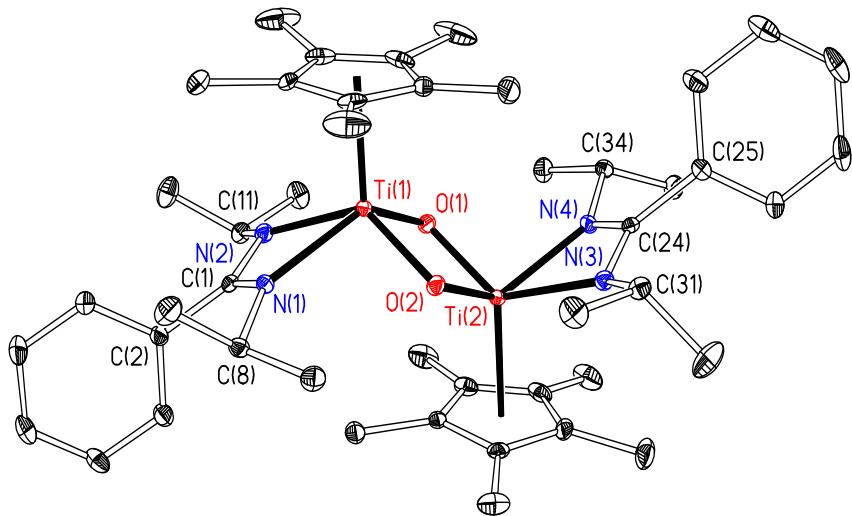
Figure S2. Displacement ellipsoid plot (20 % probability) of [Cp*Ti{PhC(N^{i}Pr)$_2$}(μ-O)]$_2$ (**23**). H atoms omitted for clarity.

Table S1. Selected bond lengths (Å) and angles (°) for [Cp*Ti{PhC(N^{i}Pr)$_2$}(μ-O)]$_2$ (**23**). Cp$_{cent(1)}$ and Cp$_{cent(2)}$ are the computed centroids for the Cp* ring carbons.

Ti(1)-Cp$_{cent(1)}$	2.138	Cp$_{cent(1)}$-Ti(1)-N(1)	107.92
Ti(2)-Cp$_{cent(2)}$	2.143	Cp$_{cent(1)}$-Ti(1)-N(2)	108.69
Ti(1)-N(1)	2.1954(19)	Cp$_{cent(2)}$-Ti(2)-N(3)	109.45
Ti(1)-N(2)	2.195(2)	Cp$_{cent(2)}$-Ti(2)-N(4)	108.00
Ti(2)-N(3)	2.215(2)	Cp$_{cent(1)}$-Ti(1)-O(1)	115.88
Ti(2)-N(4)	2.168(2)	Cp$_{cent(1)}$-Ti(1)-O(2)	118.75
Ti(1)-O(1)	1.8670(17)	Cp$_{cent(2)}$-Ti(2)-O(1)	116.00
Ti(1)-O(2)	1.8572(18)	Cp$_{cent(2)}$-Ti(2)-O(2)	118.78
Ti(2)-O(1)	1.8599(18)	N(1)-Ti(1)-N(2)	60.60(8)
Ti(2)-O(2)	1.8614(17)	N(3)-Ti(2)-N(4)	60.61(8)
		O(1)-Ti(1)-O(2)	81.17(8)
		O(1)-Ti(2)-O(2)	81.25(7)
		Ti(1)-O(1)-Ti(2)	98.64(8)
		Ti(1)-O(2)-Ti(2)	98.94(9)

25a-anti
2.7 (1.9) kcal mol^{-1}

25a-syn
0.0 kcal mol^{-1}

25b-anti
6.0 (5.6) kcal mol^{-1}

25b-syn
0.0 kcal mol^{-1}
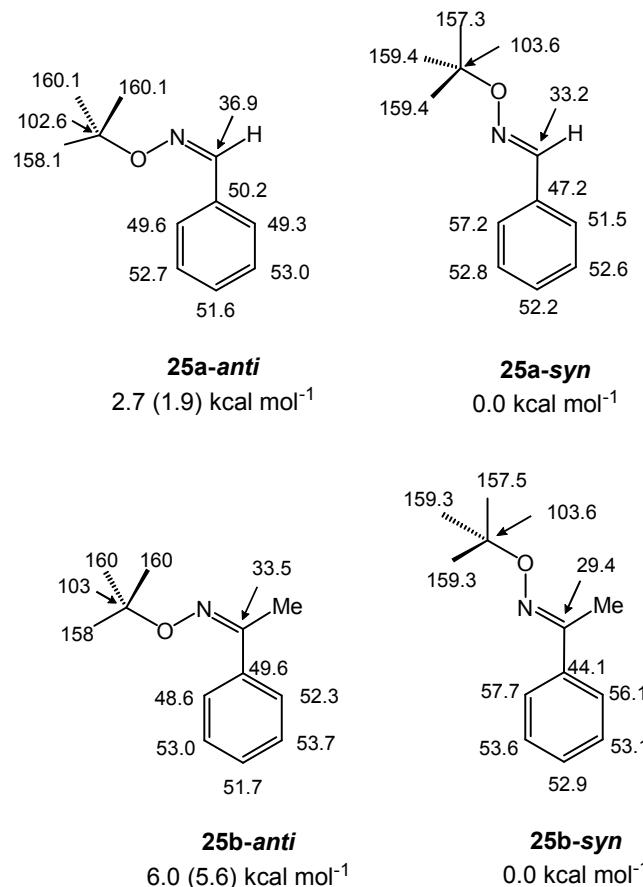
Figure S3. Computed isotropic magnetic shielding tensors and pairwise relative Gibbs free energies at 298 K (the values in parentheses include a dispersion correction) for the *anti* and *syn* isomers of PhC(NO^{t}Bu)R (R = H (**25a**) or Me (**25b**)).
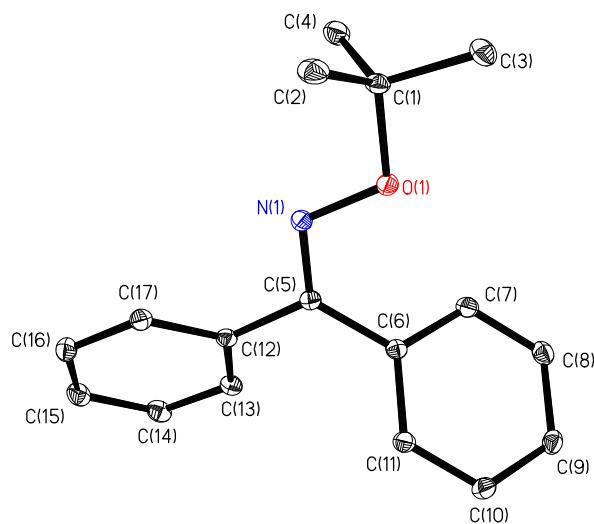

Figure S4. Displacement ellipsoid plot (20% probability) of PhC(NO^{t}Bu)Ph (**25c**). H atoms omitted for clarity.

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Table S2. Selected bond lengths (Å) and angles (°) for PhC(NO^{t}Bu)Ph (**25c**).

|			
C(1)-O(1)	1.4631(11)	N(1)-O(1)-C(1)	110.50(7)
N(1)-O(1)	1.3980(9)	C(5)-N(1)-O(1)	112.30(7)
N(1)-C(5)	1.2888(12)	C(6)-C(5)-N(1)	125.68(8)
C(5)-C(12)	1.4886(12)	C(12)-C(5)-N(1)	114.77(8)
C(5)-C(6)	1.4910(12)		
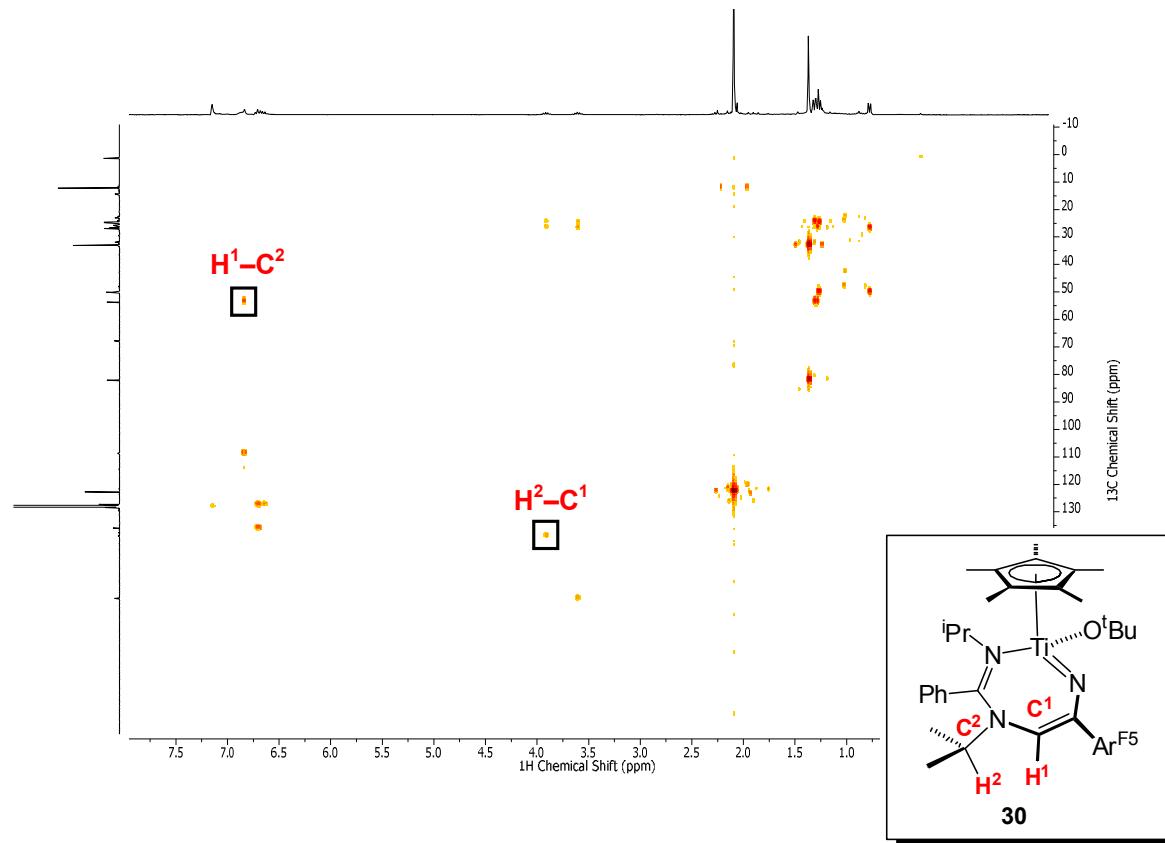
Figure S5. Gradient selective ^{1}H-^{13}C Heteronuclear Multiple-Bond Correlation (HMBC) NMR spectrum for Cp*Ti(O^{t}Bu){NC(Ar^{F_5})C(H)N(^{i}Pr)C(Ph)N(^{i}Pr)} (**30**).
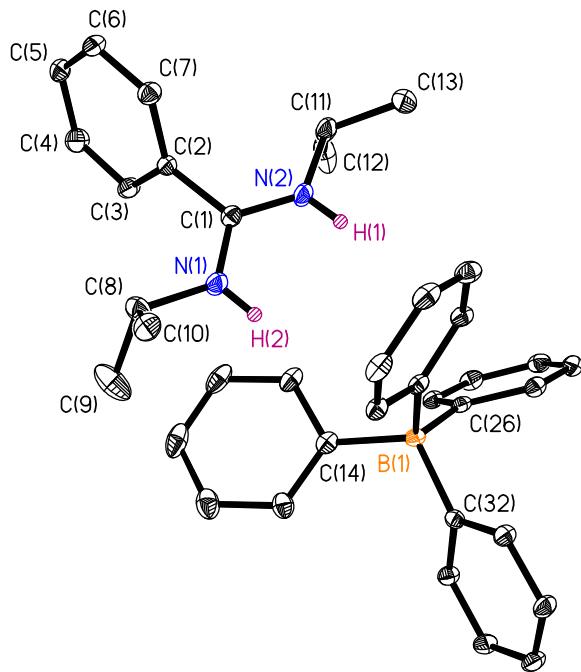
Figure S6. Displacement ellipsoid plot (20 % probability) of [PhC(N^{i}PrH)$_2$][BPh$_4$] (**33-BPh$_4$**). C-bound H atoms omitted for clarity.

Table S3. Selected bond lengths (Å) and angles (°) for [PhC(N^{i}PrH)$_2$][BPh$_4$] (**33-BPh$_4$**).

N(1)-C(1)	1.3061(17)	N(1)-C(1)-N(2)	120.16(12)
N(1)-C(8)	1.4847(17)	H(2)-N(1)-C(1)	118.4(11)
N(2)-C(1)	1.3159(17)	H(1)-N(2)-C(1)	120.1(11)
N(2)-C(11)	1.4809(18)		
C(1)-C(2)	1.4901(18)		

Table S4. X-ray data collection and processing parameters for Cp*Ti{PhC(N^{i}Pr)$_2$}(NO^{t}Bu) **(19)**, Cp*Ti{PhC(N^{i}Pr)$_2$}{OC(NTol)N(Tol)C(NO^{t}Bu)O} **(22)**, PhC(NO^{t}Bu)Ph **(25c)**, [Cp*Ti{PhC(N^{i}Pr)$_2$}(μ-O)]$_2$ **(23)**, Cp*Ti{PhC(N^{i}Pr)$_2$}{NC(Ar^{F5})NO^{t}Bu} **(26)**, Cp*Ti{PhC(N^{i}Pr)$_2$}{NC(Ar^{F5})NC(Ar^{F5})N(C{Ar^{F5}}NO^{t}Bu)} **(29)**, [PhC(N^{i}PrH)$_2$][BPh$_4$] **(33-BPh$_4$)** and Cp*Ti{PhC(N^{i}Pr)$_2$}{η^2-ON(H)B(Ar^{F5})$_3$} **(36)**.

compound	19	22	23	25c	26
empirical formula	C$_{27}$H$_{43}$N$_3$OTi	C$_{43}$H$_{57}$N$_5$O$_3$Ti	C$_{46}$H$_{68}$N$_4$O$_2$Ti$_2$	C$_{17}$H$_{19}$NO	C$_{34}$H$_{43}$F$_5$N$_4$OTi
fw	473.51	739.86	804.87	253.34	666.63
temp / K	150	150	150	150	150
wavelength / Å	0.71073	1.54184	0.71073	1.54184	0.71073
space group	$P\,2_12_12_1$	$P\,\overline{1}$	$P\,2_1/c$	$P\,2_12_12_1$	$P\,\overline{1}$
a / Å	16.6135(2)	10.8924(4)	32.0878(2)	8.46178(11)	10.6906(10)
b / Å	17.1813(2)	11.4025(4)	10.8165(1)	10.87960(15)	11.8098(11)
c / Å	19.3943(2)	18.6552(6)	26.5749(1)	15.6091(2)	13.8987(15)
α / deg	90	72.928(3)	90	90	96.244(4)
β / deg	90	79.432(3)	110.7542(3)	90	93.745(4)
γ / deg	90	68.018(3)	90	90	98.297(5)
V / Å^3	5535.94(11)	2046.79(13)	8625.03(10)	1436.99(3)	1720.2(3)
Z	8	2	8	4	2
d (calcd) / Mg.m^{-3}	1.136	1.200	1.240	1.171	1.287
abs coeff / mm^{-1}	0.331	2.109	0.411	0.562	0.308
R indices: R_1 =	0.0459^a	0.0388^a	0.0468^a	0.0298^a	0.0836^b
R_w =	0.0520^a	0.0431^a	0.0564^a	0.0322^a	0.0732^b

^{a} $R_1 = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$; $R_w = \sqrt{\{\Sigma w(|F_o|-|F_c|)^2 / \Sigma w|F_o|^2\}}$ for data with I > 3σ(I).

^{b} $R_1 = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$; $R_w = \sqrt{\{\Sigma w(|F_o|-|F_c|)^2 / \Sigma w|F_o|^2\}}$ for data with I > 2σ(I).

Table S4. (Cont.)

compound	**29**	**33·BPh$_4$**	**36·C$_6$H$_6$**
empirical formula	C$_{48}$H$_{43}$F$_{15}$N$_6$OTi	C$_{37}$H$_{41}$BN$_2$	C$_{41}$H$_{35}$BF$_{15}$N$_3$OTi·C$_6$H$_6$
fw	1052.78	524.56	1007.54
temp / K	150	150	150
wavelength / Å	0.71073	1.54180	1.54180
space group	P 2$_1$/*n*	P $\bar{1}$	P 2$_1$/*c*
a / Å	12.62440(10)	9.7572(8)	13.2439(2)
b / Å	18.3472(2)	10.1086(7)	13.8026(3)
c / Å	20.5455(2)	16.5470(11)	24.0023(3)
α / deg	90	98.985(6)	90
β / deg	97.6073(4)	105.885(6)	97.7434(15)
γ / deg	90	95.944(6)	90
V / Å^3	4716.91(8)	1532.0(2)	4347.59(13)
Z	4	2	4
d (calcd) / Mg.m^{-3}	1.482	1.137	1.539
abs coeff / mm^{-1}	0.285	0.488	2.621
R indices: R_1 =	0.0340^a	0.0581^b	0.0324^a
R_w =	0.0430^a	0.0284^b	0.0298^a

^{a} $R_1 = \Sigma||F_\text{o}|-|F_\text{c}|| / \Sigma|F_\text{o}|$; $R_\text{w} = \sqrt{\{\Sigma w(|F_\text{o}|-|F_\text{c}|)^2 / \Sigma w|F_\text{o}|^2\}}$ for data with I $> 3\sigma$(I).

^{b} $R_1 = \Sigma||F_\text{o}|-|F_\text{c}|| / \Sigma|F_\text{o}|$; $R_\text{w} = \sqrt{\{\Sigma w(|F_\text{o}|-|F_\text{c}|)^2 / \Sigma w|F_\text{o}|^2\}}$ for data with I $> 2\sigma$(I).

DFT calculations: cartesian coordinates (Å), electronic energies (a.u.), Gibbs correction at 298 K (a.u.) and D3(bj) dispersion correction (a.u.) for all the species in Fig 6.

Cp*Ti{(PhC(N^iPr)₂}(NO^tBu) (19)

E(smd) = -1352.54911130
G(298) = 0.581065
Edisp = -0.18716112

```
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N,0,1.0629893456,-0.4779948641,-0.0733689641
C,0,-1.2085409072,-2.2341023313,-0.6369048919
C,0,-1.2526180364,-1.3720522241,-1.7743013466
C,0,-2.3059708198,-0.4329249665,-1.5706561993
C,0,-2.9027511587,-0.6963785546,-0.3066940934
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C,0,-0.2631000452,-0.278649923,3.8334585936
C,0,-2.4775322138,0.9395537375,3.8134055038
C,0,-0.1413044002,3.1113471631,-0.9480250693
C,0,0.7670675063,2.5214000787,-2.0253479381
C,0,-1.2663855281,3.9468836501,-1.5655619797
H,0,-5.0100994775,-0.2519070941,-0.2468198159
H,0,-4.2119051633,-0.1785965949,1.3252764295
H,0,-3.9722419492,1.1192389803,0.1571616307
H,0,-3.5843822322,0.1459763265,-3.1931100581
H,0,-3.2233279821,1.453277506,-2.0614531022
H,0,-2.0040973663,0.9254162585,-3.2261043005
H,0,-0.3786266673,-0.5968241286,-3.5903088725
H,0,0.6266701433,-1.7765518118,-2.7485847882
H,0,-0.7979573938,-2.3080677241,-3.6583897414
H,0,-0.7114370373,-4.2866236876,-1.0457621595
H,0,0.690421479,-3.2146178533,-0.8618687718
H,0,-0.2202894288,-3.7320241328,0.5566844432
H,0,-3.30653975,-3.3231501978,1.347888646
H,0,-1.7226596376,-2.9641527018,2.029681391
H,0,-3.0615454126,-1.8373345303,2.2636876684
H,0,1.1987759554,3.3168730381,-2.6425780353
H,0,1.5744940049,1.9392805576,-1.5751669932
H,0,0.2028757696,1.8508539462,-2.6831896531
H,0,-1.8966808177,3.3312382326,-2.2137012249
H,0,-0.8516485381,4.7629426627,-2.1680763788
H,0,-1.8993915455,4.3873090123,-0.7896547449
H,0,0.4699343783,3.7873636967,-0.3333306706
H,0,-3.0080225906,1.8297664454,3.462673328
H,0,-2.5172620113,0.9277814082,4.9084984935
H,0,-3.0118820916,0.0587721114,3.4443280816
H,0,-0.6857048763,-1.2009437128,3.4210617937
H,0,0.7894851209,-0.2273167699,3.5416866119
H,0,-0.3164512421,-0.3411397677,4.9256583162
H,0,-0.5433824131,1.8338238017,3.7489126781
C,0,3.298460306,-1.190370742,0.2736716241
C,0,-0.4882773104,3.4494253399,1.9301014694
C,0,-1.5448325809,4.344034473,2.13121063
C,0,0.7882826621,3.7829432165,2.4001080527
C,0,-1.3291577563,5.5526929926,2.7916066475
H,0,-2.5378994759,4.0891166638,1.7714777093
C,0,1.0021026499,4.9932335249,3.0564772071
H,0,1.6119865651,3.0909515569,2.2470868856
C,0,-0.0558073592,5.880236693,3.2539641002
H,0,-2.1577358307,6.23888784,2.9440615839
H,0,1.9971147904,5.2433543684,3.4143883114
```

H,0,0.1122218141,6.8231583495,3.7668180328
C,0,3.7322993489,0.2263831148,0.6409968275
H,0,3.9714369827,0.7987753062,-0.2606052446
H,0,2.9258998879,0.7385708224,1.1719354718
H,0,4.6193736093,0.2025242735,1.2822997933
C,0,2.9695691414,-2.016920156,1.514038755
H,0,2.690836446,-3.0367333179,1.2317093552
H,0,3.8313038226,-2.0674919305,2.1874970296
H,0,2.1315655925,-1.5667150032,2.0520175891
C,0,4.3426971882,-1.8827889611,-0.5948096247
H,0,5.2794587056,-2.0018706314,-0.0418997884
H,0,3.9924555433,-2.8736678582,-0.8991065338
H,0,4.5427116797,-1.2960152312,-1.4961476037
O,0,2.1286077752,-1.1366041375,-0.5958944061

PhC(O)H

E(smd) = -345.536984671
G(298) = 0.079745
Edisp = -0.02454297

C,0,0.1859525588,-0.6203612687,-0.0000203865
O,0,1.3993050692,-0.670909129,0.0003081855
H,0,-0.4241245727,-1.5520206272,-0.0003308725
C,0,-0.6032274992,0.6294852185,-0.0000480206
C,0,-2.0007448609,0.569836333,-0.0004554996
C,0,0.0449417631,1.871713562,0.0003382162
C,0,-2.7496971418,1.7436345668,-0.0004878864
H,0,-2.4961490215,-0.3991759961,-0.0007658403
C,0,-0.7029306748,3.0420369762,0.0003170796
H,0,1.1309300552,1.8877688716,0.0006522794
C,0,-2.0996657638,2.9778248374,-0.0000971962
H,0,-3.8350261696,1.6993444525,-0.0008107429
H,0,-0.2046521756,4.0074165418,0.0006232433
H,0,-2.6825935965,3.8949686711,-0.0001224791

PhC(O)Me

E(smd) = -384.856961769
G(298) = 0.105870
Edisp = -0.03018715

C,0,0.1558095414,-0.6461153406,0.0001016109
O,0,1.3745945609,-0.5909148856,0.000478567
C,0,-0.6632792921,0.607221401,0.0000281948
C,0,-2.064059926,0.5986828281,-0.0001269175
C,0,0.0129427729,1.8349222506,0.00017017
C,0,-2.7748456097,1.7967226141,-0.0001485165
H,0,-2.6070182878,-0.3418932196,-0.0002156459
C,0,-0.6958513046,3.0298738118,0.0001302997
H,0,1.0984918625,1.8180423767,0.0003064889
C,0,-2.0922788214,3.0124149886,-0.0000279273
H,0,-3.8611466073,1.7819054868,-0.0002608082
H,0,-0.1638673236,3.9772201896,0.0002290843
H,0,-2.6478865218,3.9463428978,-0.0000531572
C,0,-0.5559014743,-1.9829627859,-0.0002791938
H,0,-1.1959922988,-2.0876435776,0.8826329074
H,0,-1.1964759386,-2.086990567,-0.882910651
H,0,0.1919858283,-2.7763795088,-0.0007395056

TS1 Path1 R = H

E(smd) = -1698.05846948
G(298) = 0.687921
Edisp = -0.24181811

Ti,0,0.123108484,0.6870319989,0.4093647749
N,0,0.9212745218,-0.6807201364,1.0996055267
C,0,2.2726613302,-1.999656518,2.5776132936
C,0,1.4161061653,2.7405676013,0.4446043213

C,0,1.069233344,2.4587734415,1.7928580205
C,0,-0.3413894938,2.5537201433,1.9088398623
C,0,-0.8681714404,2.945321726,0.6383096295
C,0,0.2167857463,3.0615774268,-0.2653112264
N,0,-1.3104434351,0.1070045186,-1.0943247534
N,0,-1.8174452409,-0.0277984462,1.0352635582
C,0,-2.2028049838,-0.3229173423,-0.2010475353
C,0,-1.4794824881,0.2365620127,-2.5398757592
C,0,-2.2503535042,-0.6811004334,2.270492216
H,0,-1.5905308794,-0.2543403276,3.0342382955
H,0,-0.5892118915,0.791460127,-2.8538658829
C,0,1.713565821,-0.6751198476,-1.4091819046
O,0,1.4355798504,0.5306617311,-1.4995365806
C,0,0.1660058928,3.5015415187,-1.6962470066
H,0,0.5858811257,4.5091752537,-1.8128218215
H,0,0.7414684529,2.8315997219,-2.3435101858
H,0,-0.8578840586,3.529355909,-2.0762200637
C,0,2.8089807767,2.8802099591,-0.0901425997
H,0,3.2201244807,3.8732872563,0.1382036362
H,0,3.4889947093,2.1395520673,0.3417156644
H,0,2.8294285257,2.7564356619,-1.1753012114
C,0,2.0342087549,2.2992984704,2.9262309332
H,0,2.2886201646,3.2810747573,3.3488194747
H,0,1.6231466361,1.6973800072,3.7405985308
H,0,2.9711737438,1.8349591073,2.609211188
C,0,-1.1261532205,2.4776846736,3.1815170745
H,0,-1.1931928066,3.4651185267,3.6590675354
H,0,-2.1466988563,2.1322793753,3.0020755714
H,0,-0.6670168126,1.8000204003,3.9077067537
C,0,-2.3124157804,3.2381651804,0.376974451
H,0,-2.6620636394,4.074152377,0.9959767142
H,0,-2.4877565128,3.5113498464,-0.6660648835
H,0,-2.9393122057,2.3701159269,0.6104316027
C,0,-3.6871249672,-0.3477027732,2.6958259569
H,0,-3.8797840247,0.7283804028,2.6398655474
H,0,-4.4251621809,-0.8572750179,2.0711567711
H,0,-3.8499466369,-0.6665690149,3.7317600123
C,0,-2.010940768,-2.195702442,2.288004836
H,0,-2.7083874704,-2.7189273621,1.6272422896
H,0,-0.9880590614,-2.4223926761,1.9784339452
H,0,-2.1641515728,-2.5860342671,3.3014253153
C,0,-1.4520606259,-1.0932395963,-3.3099725041
H,0,-2.3682957264,-1.6703389636,-3.1594957674
H,0,-1.3526683807,-0.8985521801,-4.3841254503
H,0,-0.6045254916,-1.71325819,-3.0027175594
C,0,-2.6957762149,1.0691561306,-2.9650560272
H,0,-2.7358186399,2.0127403063,-2.4146555072
H,0,-2.6340102375,1.3018823762,-4.0342636035
H,0,-3.6345530551,0.5347439849,-2.7954109664
C,0,-3.4640603704,-1.0638561495,-0.5469266056
C,0,-4.7052383333,-0.4168284905,-0.5086861745
C,0,-3.4200865376,-2.4151481739,-0.9113454675
C,0,-5.8743718649,-1.1030997086,-0.8326932485
H,0,-4.7515717112,0.6307590618,-0.2256210159
C,0,-4.5900431594,-3.1046970075,-1.2254088266
H,0,-2.4630791865,-2.9278584983,-0.9393539397
C,0,-5.8201373101,-2.4497373591,-1.1898340311
H,0,-6.8289275521,-0.5846461532,-0.8031792242
H,0,-4.5392691706,-4.1552466884,-1.4986055545
H,0,-6.7318990177,-2.9859962957,-1.4380099088
O,0,1.3484524045,-1.9196838485,1.4477739782
C,0,1.581561596,-1.4708505864,3.8303018678
H,0,1.2402915769,-0.4475880386,3.6601859874
H,0,0.7124283738,-2.0874224522,4.0777984156
H,0,2.2665194669,-1.4765942435,4.6843100183
C,0,3.5474600403,-1.2277026471,2.2544458026
H,0,4.2318440542,-1.2389985678,3.1088869632
H,0,4.0581558752,-1.6685959094,1.393504499
H,0,3.302742408,-0.1909185022,2.0145070713
C,0,2.5463648117,-3.4953653855,2.6899304803
H,0,3.009270393,-3.8715673285,1.7729101149
H,0,3.2239895244,-3.694550472,3.525861474
H,0,1.615623337,-4.0446016974,2.8600774301
C,0,3.0695562813,-1.2151907567,-1.5496594835
C,0,3.2552050746,-2.6008744808,-1.4530395806
C,0,4.1661138062,-0.3773355499,-1.7993714777

C,0,4.5271338074,-3.1460790606,-1.6011232911
H,0,2.3990696814,-3.2388696385,-1.2506158693
C,0,5.4335817406,-0.9244612624,-1.9500100566
H,0,4.000397005,0.6923855085,-1.8728052769
C,0,5.6141813125,-2.307476824,-1.8500500333
H,0,4.6730613626,-4.2196535367,-1.5250488386
H,0,6.2852268042,-0.2794502199,-2.1466921334
H,0,6.6075296878,-2.731883054,-1.9687918733
H,0,0.9092760164,-1.419429153,-1.3075183637

TS1 Path2 R = H

E(smd) = -1698.06098364
G(298) = 0.686586
Edisp = -0.23434917

Ti,0,-0.2394691684,-0.8442577411,0.2096492586
N,0,-1.1617711216,0.2189156983,1.1996244025
C,0,-2.9103211816,1.1915146611,2.5112590395
C,0,-1.7215419125,-2.5766848667,-0.6042771502
C,0,-1.3008662878,-2.9603641618,0.7048100555
C,0,0.0804180591,-3.2699885786,0.6452617816
C,0,0.5257571289,-3.0685936542,-0.6918469668
C,0,-0.5855014202,-2.6505582614,-1.4669452392
N,0,1.5800732933,0.0128233148,-0.5661462764
N,0,1.497682922,-0.7635001962,1.4847928849
C,0,2.2052487368,-0.0592227744,0.6082459031
C,0,2.0347979732,0.6605954649,-1.7888374419
C,0,1.6334149803,-0.757726389,2.9395205115
H,0,0.8563707558,-1.454925849,3.2756465801
H,0,1.2035278433,0.5095853062,-2.4881919465
C,0,-2.0137963741,0.6383568192,-2.1083533523
O,0,-1.0244625805,0.4369080976,-1.4049894549
C,0,-0.5605128676,-2.4174553506,-2.9487829877
H,0,-0.4469171756,-3.3621377282,-3.4957174139
H,0,-1.4831510487,-1.9525661117,-3.3063140857
H,0,0.268521577,-1.767748359,-3.2485446501
C,0,-3.1583122855,-2.4086349818,-1.0116985114
H,0,-3.7390520296,-3.3021113903,-0.7491865315
H,0,-3.6521903328,-1.557446609,-0.5306026051
H,0,-3.2577091548,-2.2848023372,-2.0944756469
C,0,-2.210956019,-3.1865840962,1.8731410328
H,0,-2.6073777664,-4.2117068569,1.8717770645
H,0,-1.6948706116,-3.0406785714,2.826520314
H,0,-3.0669544781,-2.5070093139,1.8557248637
C,0,0.9057260005,-3.8803613278,1.7325538233
H,0,0.9432460723,-4.9724261298,1.6179373216
H,0,1.9329088771,-3.5092278667,1.7080284165
H,0,0.4984326947,-3.6754924593,2.7261740549
C,0,1.9095926967,-3.3570149021,-1.1826451165
H,0,2.0309277394,-3.0735485027,-2.2311831277
H,0,2.6645271448,-2.8165304681,-0.601060347
H,0,2.1427115767,-4.4272383017,-1.1052139673
C,0,2.9654853389,-1.2977459639,3.4793624009
H,0,3.2355940979,-2.2468844839,3.0075022457
H,0,3.7864938609,-0.593891023,3.3238130274
H,0,2.8769843886,-1.471094817,4.5580484979
C,0,1.3054678864,0.6003219331,3.5740641668
H,0,2.1129496804,1.3189755345,3.4037697521
H,0,0.3808321742,1.0045840816,3.1568918347
H,0,1.1867562645,0.4912230446,4.6588952593
C,0,2.220356489,2.1809456257,-1.6677386842
H,0,3.1550934099,2.4376270427,-1.1627976874
H,0,2.2426044328,2.6396676354,-2.6631480638
H,0,1.3965101696,2.6218907722,-1.0989308408
C,0,3.2718210194,0.01601738,-2.4281037911
H,0,3.1363273199,-1.0622363858,-2.5434389197
H,0,3.4485190729,0.4460950794,-3.4209830039
H,0,4.1697683632,0.1861353725,-1.8275230435
C,0,3.5466912252,0.5534506251,0.9048402289
C,0,4.7056228881,-0.2214151565,0.7693628044
C,0,3.6707041313,1.8828558246,1.3249710252
C,0,5.9596055695,0.3200774213,1.0449737399

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H,0,4.620051119,-1.256314265,0.4504215131
C,0,4.9247665453,2.4232077127,1.606385953
H,0,2.7800441555,2.4954932462,1.4282727185
C,0,6.0725390194,1.6443415632,1.4662505627
H,0,6.8486430998,-0.2948065562,0.9333183951
H,0,5.0038231306,3.45605466,1.934938713
H,0,7.049437341,2.0669240457,1.6845233531
O,0,-1.6536520233,1.3307182647,1.7779248098
C,0,-2.7021379658,0.2581018084,3.7000498981
H,0,-2.347886846,-0.7152100299,3.3531180169
H,0,-1.958341697,0.6715434221,4.3875524649
H,0,-3.6390486636,0.1154445659,4.2485549864
C,0,-3.9983943199,0.6790194968,1.5749937743
H,0,-4.9523378909,0.5888584804,2.1042277799
H,0,-4.1312112297,1.3638971005,0.7314778975
H,0,-3.7190891331,-0.3029535627,1.1865966543
C,0,-3.1969655924,2.6178084176,2.9669190436
H,0,-3.3169602751,3.2806250724,2.1047562401
H,0,-4.1149675603,2.6503774149,3.561744861
H,0,-2.3730754665,2.9951547702,3.5796465787
C,0,-2.3007040501,1.9043280629,-2.7811986421
C,0,-3.4239931952,1.9855963865,-3.6180271058
C,0,-1.4858500036,3.0326991738,-2.5978837611
C,0,-3.7263616362,3.1759821673,-4.2704270146
H,0,-4.0563876729,1.1107011691,-3.753081775
C,0,-1.7936433694,4.2202267513,-3.2476111694
H,0,-0.628252669,2.9557911328,-1.9386689717
C,0,-2.9111421727,4.2931781205,-4.084811188
H,0,-4.5950640981,3.236293147,-4.9194854072
H,0,-1.1663119249,5.0951731884,-3.1033429733
H,0,-3.1476688176,5.2250337398,-4.5910769922
H,0,-2.7597487555,-0.1591215251,-2.2516792525

Intermediate Path1 R = H (25a_int_H$_{down}$)

E(smd) = -1698.08879103
G(298) = 0.692166
Edisp = -0.24483088

Ti,0,0.1206448733,0.9336877899,0.3455486873
N,0,1.3609067762,-0.5740362384,0.2083670294
C,0,2.2858503068,-2.4142544823,1.4673516131
C,0,1.0499208904,3.1491471329,0.6671950267
C,0,1.1518061684,2.4133047159,1.8855584672
C,0,-0.1699707155,2.1963430438,2.3695768257
C,0,-1.0842231539,2.7862912566,1.446263451
C,0,-0.3253876454,3.3752201661,0.3996638805
N,0,-1.5192316531,0.6466060879,-0.8914598401
N,0,-1.4932866764,-0.3510556195,1.0623116002
C,0,-2.1140873247,-0.2568307789,-0.1076556859
C,0,-1.82106228,1.0341217282,-2.2668972731
C,0,-1.803833525,-1.276779675,2.1524283844
H,0,-1.0334750887,-1.0642707995,2.9014915973
H,0,-1.0836481159,1.8155035714,-2.477120387
C,0,1.6652295057,-0.2535297652,-1.1848060706
O,0,1.1821416231,1.074239027,-1.2115517851
C,0,-0.8314746486,4.1764605989,-0.7596988083
H,0,-0.7184570112,5.2513021103,-0.5656537944
H,0,-0.2716799783,3.954194394,-1.6733841657
H,0,-1.8885407921,3.9915137129,-0.9616470195
C,0,2.1774251516,3.6949211457,-0.1502387517
H,0,2.0763869689,4.7805580361,-0.2663833175
H,0,3.1425425189,3.5084361591,0.3282601045
H,0,2.2010482586,3.2431713923,-1.1474347347
C,0,2.4286636579,2.0960650083,2.6063988401
H,0,2.8227563097,2.9921765404,3.1035648942
H,0,2.2805930652,1.3390105095,3.3803981072
H,0,3.2033247938,1.7256896218,1.9297883256
C,0,-0.5301459558,1.609739882,3.6997971592
H,0,-0.4762433643,2.3770696195,4.4835831116
H,0,-1.5463026917,1.2113894538,3.7013816454
H,0,0.1453520021,0.8017290138,3.9961343757
C,0,-2.5698991144,2.848087091,1.6175873256
H,0,-2.8397114257,3.4382939934,2.5021841528

S20

H,0,-3.0521442878,3.3153229495,0.7558365119
H,0,-3.0001218239,1.8497092522,1.7426071286
C,0,-3.1567437868,-1.0211420911,2.8314947775
H,0,-3.2807849311,0.0295432524,3.1093769531
H,0,-3.991323507,-1.3025439666,2.1844007197
H,0,-3.2285109146,-1.6209273848,3.7458045614
C,0,-1.6613704463,-2.7594046476,1.7852055682
H,0,-2.5102209491,-3.1123933136,1.1940769199
H,0,-0.7421942277,-2.9147295605,1.2168206464
H,0,-1.6219171573,-3.3656726793,2.6979675194
C,0,-1.5785696539,-0.0697472383,-3.3033256576
H,0,-2.3088458058,-0.8785155669,-3.2153846071
H,0,-1.6623165761,0.3478793653,-4.3129359388
H,0,-0.5746625481,-0.4864902681,-3.1942539627
C,0,-3.2110334972,1.6578620205,-2.4468572047
H,0,-3.4074199153,2.4122876311,-1.6795002965
H,0,-3.273469157,2.1455310028,-3.4259423139
H,0,-4.0047683094,0.9080355217,-2.3971091011
C,0,-3.320196969,-1.0512587674,-0.5210424683
C,0,-4.6093740195,-0.5690856457,-0.2656623776
C,0,-3.1727730682,-2.2782016572,-1.1790099382
C,0,-5.7291753373,-1.3012808359,-0.6566418409
H,0,-4.734059598,0.3848496824,0.2385178944
C,0,-4.2932578976,-3.008785871,-1.5702774585
H,0,-2.1764020822,-2.6617172989,-1.3774833706
C,0,-5.573716082,-2.5229517814,-1.309866998
H,0,-6.7235784975,-0.9148838794,-0.4507470167
H,0,-4.1637440914,-3.9601556571,-2.0787622401
H,0,-6.4464332651,-3.093508911,-1.6149181394
O,0,1.3365969379,-1.9550658343,0.4656115332
C,0,1.8634324516,-1.9125742905,2.8477292527
H,0,1.8248881166,-0.8198241193,2.8489869835
H,0,0.8791468907,-2.3016995681,3.1207324682
H,0,2.5813572358,-2.228492134,3.6120006727
C,0,3.7139905323,-1.9781445051,1.1571256539
H,0,4.3947141611,-2.3865414294,1.9117900212
H,0,4.0316109837,-2.3348908872,0.1746284388
H,0,3.8003328985,-0.8899496434,1.1680836916
C,0,2.1635182679,-3.9341906249,1.3773330958
H,0,2.447294886,-4.2807432614,0.3794036167
H,0,2.8231730466,-4.4094705556,2.1099524805
H,0,1.138647412,-4.2585264495,1.5784659554
C,0,3.1109878898,-0.3471933835,-1.635600545
C,0,3.5071091489,-1.3890004702,-2.4766693631
C,0,4.0656360616,0.5851622259,-1.2209370519
C,0,4.8365330137,-1.5126711812,-2.8826211037
H,0,2.7668473381,-2.1112492,-2.8148375201
C,0,5.3916699158,0.4703043108,-1.6275535861
H,0,3.7531415974,1.4036286139,-0.5813127156
C,0,5.7826940864,-0.5827292824,-2.4571357748
H,0,5.1304029752,-2.3303570564,-3.5357816627
H,0,6.1244749844,1.2039481123,-1.3007349789
H,0,6.8181199836,-0.6719416795,-2.7750563152
H,0,1.0712702063,-0.9076053868,-1.8484006382

Intermediate Path2 R = H (25a_int_H~up~)

E(smd) = -1698.08566495
G(298) = 0.690609
Edisp = -0.24503678

Ti,0,-0.484188941,-0.3863181723,0.0064554407
N,0,1.4534934267,-0.4195820794,-0.0217300988
C,0,3.6374774187,-0.7764604422,-1.0838861481
C,0,-1.2691734233,-2.6193806443,-0.1342105093
C,0,-1.1096856688,-2.1677082705,-1.4773092841
C,0,-2.0750547966,-1.1493275521,-1.7078650148
C,0,-2.832309479,-0.9712146984,-0.5174298067
C,0,-2.3308156741,-1.8755537172,0.4584595551
N,0,-1.2763864491,1.2696549726,0.9921010057
N,0,-0.5931369344,1.473183225,-1.0841744953
C,0,-1.0245353767,2.1202948614,-0.0043810904
C,0,-1.6284882077,1.5390878046,2.3867900108
C,0,-0.1636077076,2.0382115322,-2.3616233813

S21

H,0,-0.0507260693,1.1618422569,-3.0117171595
H,0,-1.5152597686,0.5602786238,2.8653458153
C,0,1.578388743,-0.8214137745,1.3660893754
O,0,0.2068029561,-0.998515292,1.6703917301
C,0,-2.8055920802,-2.0577565101,1.8669508169
H,0,-3.3099651387,-3.0243104953,1.9907316309
H,0,-1.9632291406,-2.0313494755,2.566487902
H,0,-3.5109806296,-1.277271563,2.1620492959
C,0,-0.5231068849,-3.7307216088,0.5335629908
H,0,-1.1182034954,-4.6532051206,0.5391036769
H,0,0.4175085207,-3.9510209399,0.0215774723
H,0,-0.2868873629,-3.4694260385,1.5684718223
C,0,-0.2558617462,-2.7942726403,-2.5369361696
H,0,-0.8443626118,-3.513186902,-3.1225671273
H,0,0.1394033439,-2.054894953,-3.240066143
H,0,0.5912053754,-3.3356244184,-2.1135533262
C,0,-2.3937575738,-0.5315533772,-3.0321094587
H,0,-3.1114305557,-1.1569932302,-3.5805918883
H,0,-2.8414426266,0.4572315628,-2.9167298938
H,0,-1.510049969,-0.4276933255,-3.6674318018
C,0,-4.0158363788,-0.0620936178,-0.4043302011
H,0,-4.7573906287,-0.2981702643,-1.1772111189
H,0,-4.5120698013,-0.1664597383,0.5628690725
H,0,-3.7383972297,0.9907025609,-0.524968938
C,0,-1.1841744882,2.9623304702,-3.0407712142
H,0,-2.1877264079,2.52801462,-3.0397323487
H,0,-1.236358014,3.9386866499,-2.5533916499
H,0,-0.8884055817,3.1271978314,-4.0828396679
C,0,1.2133669478,2.7118135344,-2.3024638615
H,0,1.1633545041,3.6648068717,-1.7678155279
H,0,1.9340674576,2.0580289432,-1.8077632356
H,0,1.5680204055,2.9223411292,-3.3184609302
C,0,-0.6852807521,2.4931484757,3.1264615038
H,0,-0.8184409696,3.5304831741,2.8080525214
H,0,-0.8969698819,2.4468108439,4.2005162532
H,0,0.3576685547,2.2084588885,2.9767418405
C,0,-3.0860642093,1.978118199,2.5724894032
H,0,-3.7773015234,1.2905601331,2.0801665514
H,0,-3.3319249845,2.000778679,3.6400849843
H,0,-3.2549585715,2.9819376259,2.1716398848
C,0,-1.212152705,3.6068508535,0.0943817045
C,0,-2.4782394647,4.1715338334,-0.1008295261
C,0,-0.132616452,4.4485530365,0.3864728721
C,0,-2.6590586961,5.5509101246,-0.0180065379
H,0,-3.3227247019,3.5278448363,-0.3293457339
C,0,-0.3149993315,5.8274918271,0.4722833305
H,0,0.8475168274,4.0174864397,0.5642808906
C,0,-1.5773845559,6.3826161611,0.2672308225
H,0,-3.6466456626,5.9750520785,-0.1771501702
H,0,0.5314133389,6.4683553136,0.703377085
H,0,-1.7179637709,7.4578980968,0.3326045803
O,0,2.5450344308,0.115046725,-0.7056450278
C,0,3.1195035447,-2.0867577532,-1.6570812105
H,0,2.5304652653,-2.6319318905,-0.9152067808
H,0,2.4908647789,-1.9036883948,-2.5314009897
H,0,3.9605631683,-2.7183604049,-1.9610211199
C,0,4.5808953794,-1.0236147147,0.0975011304
H,0,5.4844627595,-1.5362235276,-0.2506063365
H,0,4.8770587771,-0.0776805923,0.5577731342
H,0,4.1234723562,-1.6490984626,0.8675143944
C,0,4.3599902456,0.0379496976,-2.1565177012
H,0,4.6798758121,1.0027709055,-1.7516444433
H,0,5.2466324316,-0.4972948737,-2.5097264131
H,0,3.7006084069,0.2236459742,-3.0089254767
H,0,2.0711454905,-1.8092070937,1.4669739099
C,0,2.2618482113,0.1317897044,2.3325763537
C,0,2.4704630057,-0.3110399072,3.6436256813
C,0,2.6821446883,1.4172909902,1.9800309805
C,0,3.0709284243,0.5147171207,4.5897634283
H,0,2.1486687964,-1.3120999577,3.922467432
C,0,3.2995790521,2.2406502978,2.9240063744
H,0,2.547310547,1.7576805661,0.9596918481
C,0,3.4915811212,1.7957757709,4.2302449079
H,0,3.217321919,0.1579186387,5.606025496
H,0,3.6322634314,3.2347477962,2.6353893272
H,0,3.9707441603,2.4395726973,4.9630719889

TS2 Path1 R = H

E(smd) = -1698.06410413
G(298) = 0.691098
Edisp = -0.24538727

Ti,0,-0.2857204193,-0.6443968514,0.2097519739
N,0,-1.6181531149,1.3030352187,0.0602534756
C,0,-1.5345803561,3.6856339031,0.1400873631
C,0,-1.8724102079,-1.1727685421,2.0067593801
C,0,-0.6210105954,-1.0240489597,2.6781228201
C,0,0.2532650512,-2.0242980343,2.1964810915
C,0,-0.4566118174,-2.790654394,1.2153534646
C,0,-1.7772025249,-2.2794356566,1.1166736384
N,0,1.5959527457,-1.3394069417,-0.5185474358
N,0,1.4458029118,0.583571359,0.5253942407
C,0,2.2225143607,-0.2053732023,-0.2139797958
C,0,1.8713804696,-2.2176285392,-1.659778364
C,0,1.8686294748,1.7537826724,1.2946692376
H,0,0.9350742148,2.1396795312,1.7148283941
H,0,1.0330104096,-2.9215072858,-1.6504096106
C,0,-1.9462882321,0.8352506838,-1.1479950185
O,0,-0.8885033035,-0.8249188492,-1.3715606876
C,0,-2.880082387,-2.8900643607,0.3081772799
H,0,-3.6997704453,-2.1890272599,0.1391466013
H,0,-2.5225710174,-3.2100322816,-0.6744034582
H,0,-3.2924055298,-3.7706405698,0.8184495554
C,0,-3.1106875328,-0.427122885,2.3929520142
H,0,-3.4090381482,-0.7046969022,3.4129933689
H,0,-2.9554141203,0.6546694765,2.3726287159
H,0,-3.947239048,-0.6617780906,1.7330976807
C,0,-0.3751810778,-0.0225270444,3.7650799946
H,0,-1.1122662728,-0.1398556253,4.5694320257
H,0,0.613878703,-0.1420487641,4.2125721171
H,0,-0.45635117,1.0099742399,3.4073393279
C,0,1.6495642513,-2.3195850488,2.6442435466
H,0,1.7226992813,-3.3378678351,3.0457958049
H,0,2.3526846547,-2.2447401371,1.8067581401
H,0,1.98016996,-1.6342333624,3.4279526225
C,0,0.0361155073,-4.0559322493,0.5857291882
H,0,-0.2012235511,-4.9171760547,1.2253776815
H,0,-0.4326361117,-4.2386671937,-0.3854338717
H,0,1.1190698093,-4.043260175,0.4444261805
C,0,2.7994688727,1.3973803889,2.4598277703
H,0,2.381906404,0.5941749676,3.0697564206
H,0,3.7824241663,1.0796471048,2.0987118355
H,0,2.9494839437,2.2718440516,3.1034496492
C,0,2.4744030946,2.8940750801,0.4674078142
H,0,3.5003673377,2.6798816302,0.1603354564
H,0,1.8698534253,3.0860448003,-0.4208486947
H,0,2.4987965403,3.808409755,1.0712370056
C,0,1.8186632645,-1.5165225465,-3.0220382862
H,0,2.6872290849,-0.8714612892,-3.1815088372
H,0,1.8116469543,-2.2643215443,-3.8236139693
H,0,0.9049031382,-0.9223005747,-3.0959276424
C,0,3.1517923242,-3.0490823607,-1.50891997
H,0,3.199627026,-3.5301722707,-0.5267240576
H,0,3.1724798015,-3.835481654,-2.2718561466
H,0,4.0512858051,-2.4406942367,-1.6332508757
C,0,3.6249434367,0.1144080249,-0.6482416841
C,0,4.7113035619,-0.4451016551,0.0346325958
C,0,3.8726040604,0.9540953726,-1.7408183574
C,0,6.0183820093,-0.1645115,-0.3607633552
H,0,4.5299602258,-1.1049946973,0.8782839894
C,0,5.1786367872,1.2247819068,-2.1431377102
H,0,3.0369361024,1.4000637976,-2.2716466864
C,0,6.2551828291,0.6687320725,-1.4526564301
H,0,6.8511482511,-0.6020346865,0.1830114917
H,0,5.3550480788,1.8749010208,-2.9956854414
H,0,7.2734192587,0.8838156236,-1.7645824568
O,0,-0.784205848,2.4693585551,-0.1075108242
C,0,-2.1416349437,3.6777656726,1.5434122857
H,0,-2.888662181,2.888063593,1.6441930864

H,0,-1.3625356052,3.5117412646,2.2937314749
H,0,-2.6234677169,4.63836053,1.7540483509
C,0,-2.6139125032,3.8984129403,-0.9254617296
H,0,-3.1050589527,4.8651597511,-0.7726831252
H,0,-2.1710069497,3.899215479,-1.9268714169
H,0,-3.3863509922,3.1270264293,-0.8881958647
C,0,-0.4835276903,4.787401678,0.0264396242
H,0,0.0067644858,4.7549486198,-0.9508769994
H,0,-0.9577837927,5.7669382535,0.1410494221
H,0,0.2792616663,4.6814066296,0.8008160645
C,0,-3.2727908823,0.2179942778,-1.4182276756
C,0,-3.4704702091,-0.580598751,-2.5535784862
C,0,-4.3745720366,0.5534831322,-0.6242836158
C,0,-4.7390094884,-1.0538576713,-2.8673968548
H,0,-2.6124939648,-0.8467105789,-3.1614137995
C,0,-5.646726044,0.0736049059,-0.9377342331
H,0,-4.2238147493,1.1993099862,0.2335197826
C,0,-5.83158784,-0.7329761385,-2.0576215408
H,0,-4.8786057577,-1.6785890448,-3.7454425948
H,0,-6.4931053661,0.3403404994,-0.3105231042
H,0,-6.82229924,-1.1036989144,-2.3063241465
H,0,-1.4791380045,1.3291013313,-2.002196191

TS2 Path2 R = H

E(smd) = -1698.07032111
G(298) = 0.688389
Edisp = -0.24458361

Ti,0,0.1140198739,1.0502394782,-0.2979860256
N,0,1.9018834533,0.1572228854,0.7254947102
C,0,2.7219720701,-1.3408854583,2.3875804889
C,0,1.3021487305,3.082460288,0.3393413401
C,0,0.1227667365,3.0582429779,1.1495480262
C,0,-0.9967718854,3.1545994988,0.2924423502
C,0,-0.5128788218,3.2224315781,-1.0539706004
C,0,0.9056794224,3.2053625155,-1.0217525989
N,0,-1.7577820051,0.4128081138,-1.0913238005
N,0,-1.1642248477,-0.1036800451,0.9537963148
C,0,-2.0289465783,-0.3445487138,-0.0289643696
C,0,-2.1310742367,0.1466812964,-2.4844247569
C,0,-1.2656413029,-0.5182486644,2.3507549879
H,0,-0.3574759514,-0.1124022327,2.8055946068
H,0,-1.5850622665,0.9110024969,-3.0467795959
C,0,2.3793011569,0.0826434296,-0.5441257257
O,0,0.9134375108,0.3357764971,-1.6477302251
C,0,1.7924211701,3.3324761227,-2.2231495699
H,0,2.8506118839,3.3061725612,-1.9489044775
H,0,1.6164188831,2.518022904,-2.9340683642
H,0,1.6185258632,4.2829114083,-2.7414166418
C,0,2.6948099831,3.1594821547,0.886882143
H,0,2.8150738069,4.0677312029,1.4904331181
H,0,2.9258147797,2.2973705811,1.5187525057
H,0,3.4437811952,3.2024565214,0.0912828866
C,0,0.1353969293,3.0132896758,2.6458904954
H,0,0.5488732827,3.9413766187,3.0619643449
H,0,-0.8676874664,2.889595203,3.0600402968
H,0,0.7534080038,2.1904540371,3.0186679096
C,0,-2.4415025994,3.2409002361,0.6716535507
H,0,-2.8634383699,4.2101110894,0.3778393587
H,0,-3.0262079898,2.4616238795,0.1706859331
H,0,-2.5861093036,3.1347886683,1.7488005208
C,0,-1.3492242477,3.4879480171,-2.266006208
H,0,-1.500380271,4.5683237405,-2.3965286043
H,0,-0.8717754587,3.1167073203,-3.1771940428
H,0,-2.3366687441,3.0276266666,-2.1863828391
C,0,-2.4622620554,0.1068029038,3.0780743712
H,0,-2.4903685923,1.1898644895,2.9373548984
H,0,-3.4085869163,-0.3092925532,2.7198954462
H,0,-2.3957041425,-0.0955864065,4.1530722499
C,0,-1.2304562621,-2.0336792885,2.5789413939
H,0,-2.1803898372,-2.5092561839,2.3235085266
H,0,-0.4341376291,-2.485623471,1.985065133
H,0,-1.032734339,-2.2403304323,3.6373709224

C,0,-1.6394532329,-1.203073208,-3.0191765453
H,0,-2.1978356557,-2.0388108116,-2.5873351715
H,0,-1.7758601814,-1.2426553765,-4.1060337787
H,0,-0.5754660474,-1.3235272658,-2.8023228284
C,0,-3.6210464487,0.3597598939,-2.7806021007
H,0,-3.974509156,1.311506641,-2.3710453873
H,0,-3.7812949896,0.3771229114,-3.8644033911
H,0,-4.2398679817,-0.4396039319,-2.3653469248
C,0,-3.168757226,-1.3202979864,0.0384127528
C,0,-4.4682460891,-0.8568190627,0.2765750754
C,0,-2.9622183827,-2.6925213243,-0.1452697291
C,0,-5.5382151758,-1.7480234577,0.3374673042
H,0,-4.6394260844,0.2071069446,0.4130339638
C,0,-4.0338437089,-3.581684543,-0.0955360607
H,0,-1.95723374,-3.0625125631,-0.3239918316
C,0,-5.3239849128,-3.1123633735,0.1485489359
H,0,-6.5403312161,-1.374149303,0.5286114725
H,0,-3.8589674136,-4.6436105642,-0.2447338788
H,0,-6.1582780358,-3.8069337767,0.1911295825
O,0,1.7623562386,-1.1389310427,1.3155755682
C,0,2.4263536973,-0.408330748,3.5624491251
H,0,2.504437135,0.6354411594,3.2484951786
H,0,1.421706834,-0.5832437262,3.9575153403
H,0,3.1438494005,-0.5754684052,4.3727926561
C,0,4.1632880663,-1.1456172217,1.9113411933
H,0,4.8529525081,-1.3585045743,2.7349297353
H,0,4.3995946199,-1.8178343251,1.0829162334
H,0,4.3357119984,-0.1162333555,1.5866663773
C,0,2.5027039842,-2.800477859,2.7810417713
H,0,2.6798842517,-3.4562296075,1.923613727
H,0,3.1952659212,-3.0815930438,3.5805316926
H,0,1.4830722651,-2.9622660528,3.138786535
H,0,2.8469085269,1.0162876481,-0.8536158699
C,0,2.9826325041,-1.1069131906,-1.202247855
C,0,4.2042780744,-0.9361185286,-1.8610461021
C,0,2.3756605984,-2.3696479149,-1.210460519
C,0,4.8296773457,-2.0096911095,-2.4933081844
H,0,4.6731553921,0.044974704,-1.8747696257
C,0,2.995109419,-3.4374045775,-1.8512942575
H,0,1.4209557069,-2.5011127343,-0.7175484373
C,0,4.2258989008,-3.2643517255,-2.4882675817
H,0,5.7820226864,-1.861633857,-2.9948953012
H,0,2.5149417834,-4.4123708415,-1.8559860539
H,0,4.7059122048,-4.1034365211,-2.9846031885

Cp*Ti{(PhC(N^{i}Pr)$_2$}(O)

E(smd) = -1140.04816243
G(298) = 0.460053
Edisp = -0.15430166

Ti,0,-0.2029327771,-1.166136234,-0.5247769213
C,0,-1.919259374,-2.706118767,-1.0393281928
C,0,-1.3265254075,-3.1593774192,0.175285848
C,0,0.0035098281,-3.604868882,-0.1126935542
C,0,0.2468881929,-3.3863837341,-1.4905777096
C,0,-0.9343379711,-2.8099637028,-2.0616211611
N,0,1.6928146801,-0.5235859791,-1.0728699978
N,0,1.09275742,-0.7540977701,1.0494453852
C,0,1.9882899298,-0.2417220289,0.2016338166
C,0,2.2505261217,0.0594177626,-2.2933059197
C,0,0.9942602258,-0.6007641338,2.4991580388
H,0,0.2001665625,-1.3049415046,2.7789491142
H,0,1.7429994208,-0.4924364671,-3.0952703641
O,0,-1.2245340133,0.0924133142,-0.716993567
C,0,-1.1441336052,-2.4635014727,-3.5074406174
H,0,-1.5348897366,-3.3235805232,-4.0669231124
H,0,-1.8607890013,-1.6455023601,-3.6223905273
H,0,-0.2137213845,-2.1597832709,-3.9974550242
C,0,-3.320967847,-2.2116045684,-1.2265681914
H,0,-3.9426071758,-2.9675498086,-1.7229975536
H,0,-3.7930273047,-1.9737985515,-0.2701431854
H,0,-3.3445731856,-1.2986350167,-1.8284209373
C,0,-2.0172261512,-3.2618009843,1.5050799933
H,0,-2.5163164488,-4.2332945583,1.6156600316

H,0,-1.3159451189,-3.1673577198,2.340134729
H,0,-2.7817202352,-2.4892652156,1.6277005107
C,0,0.9553650604,-4.22862556,0.8613793132
H,0,0.8590337652,-5.322472018,0.8679905524
H,0,1.9958186452,-3.9955993072,0.6156620311
H,0,0.7745822375,-3.8827997662,1.8828350853
C,0,1.4976828088,-3.7471775061,-2.2321520813
H,0,1.4643927084,-4.7872142143,-2.5825072852
H,0,1.6434758461,-3.11595309,-3.1131790969
H,0,2.3860341219,-3.6410994233,-1.602912646
C,0,2.2409480384,-1.0293125483,3.2803695934
H,0,2.5947596533,-2.008641289,2.9441323464
H,0,3.0588550153,-0.3125989548,3.1785258269
H,0,1.9942680967,-1.1046869944,4.3449913881
C,0,0.5071843101,0.7911950426,2.9184012231
H,0,1.2871745523,1.5443497371,2.7742690883
H,0,-0.3707674824,1.0831065329,2.3347406629
H,0,0.2343342962,0.791558918,3.979556187
C,0,1.8752031287,1.5348131995,-2.4722375331
H,0,2.4286173205,2.1712671333,-1.7753940363
H,0,2.1158940111,1.8654100827,-3.4887068173
H,0,0.8042049731,1.6800956616,-2.3030166471
C,0,3.7504333677,-0.180266237,-2.4951102781
H,0,4.0025839427,-1.2325952358,-2.3323604834
H,0,4.0246524272,0.0793291853,-3.523440711
H,0,4.3595845437,0.4295032733,-1.8241534933
C,0,3.1881847039,0.5531777078,0.6257823763
C,0,4.4170810899,-0.0885568547,0.8214892884
C,0,3.0980191987,1.934170652,0.8313165643
C,0,5.5358235937,0.6394356438,1.2198173097
H,0,4.4931085659,-1.1601195435,0.6616780565
C,0,4.2202300187,2.6610621492,1.2271047365
H,0,2.1488471381,2.4387953708,0.6775948089
C,0,5.4399521024,2.0159326722,1.4235299235
H,0,6.4838179257,0.1304887075,1.3705092781
H,0,4.138792402,3.7333154187,1.3817504442
H,0,6.3131750589,2.5830835303,1.7332982835

Ph(CNO^tBu)H anti (25a_*anti*)

E(smd) = -558.073673496
G(298) = 0.199443
Edisp = -0.04995963

C,0,0.5172265828,1.2441716043,-0.0130033324
H,0,-0.0527851235,0.3146249777,-0.0128763468
C,0,-0.2891914396,2.4679599969,-0.0131726858
C,0,-1.6859940021,2.2969999789,-0.0131885399
C,0,0.2215025607,3.7793835717,-0.0133147556
C,0,-2.5462802023,3.3882489948,-0.0133432458
H,0,-2.0955600693,1.2893157015,-0.0130785823
C,0,-0.6445943263,4.8691232388,-0.0134673266
H,0,1.2916252384,3.9322268008,-0.0132989153
C,0,-2.0264391354,4.6824919202,-0.0134839805
H,0,-3.6212240817,3.2301463825,-0.0133537736
H,0,-0.2340520016,5.8753475161,-0.0135744251
H,0,-2.6942536261,5.5396145835,-0.0136050766
N,0,1.7827355785,1.0166861877,-0.0129737629
O,0,2.5681137118,2.1446132388,-0.0131337184
C,0,3.9821195058,1.7978625223,-0.0130863807
C,0,4.3148263736,1.0093334211,1.2513114156
C,0,4.31482465,1.0089768117,-1.2772622705
C,0,4.6678484429,3.1598670373,-0.0132792283
H,0,4.0495456102,1.5863337956,2.1426124941
H,0,3.7607240622,0.0679886789,1.2697231718
H,0,5.3857927662,0.7862123794,1.289852074
H,0,4.0495362298,1.5857227665,-2.1687255499
H,0,5.3857921805,0.7858512123,-1.3157442504
H,0,3.7607279537,0.0676233701,-1.2954054664
H,0,5.7545860107,3.0347465667,-0.0132574413
H,0,4.3872023523,3.7338711765,-0.90152629
H,0,4.3871962277,3.7341243674,0.8748020999

Ph(CNO^tBu)H syn (25a_*syn*)

E(smd) = -558.077027320
G(298) = 0.198545
Edisp = -0.04872955

C,0,-0.4701116674,-1.7235017279,0.0001770902
H,0,-0.7129059984,-2.7899250947,0.0002861002
C,0,-1.5737743333,-0.7634441078,0.0000135662
C,0,-2.8903453236,-1.2451347355,-0.000007876
C,0,-1.360307355,0.6252261428,-0.0001184775
C,0,-3.969580113,-0.3650127426,-0.0001572217
H,0,-3.0656052878,-2.3185205325,0.0000943028
C,0,-2.4385940798,1.5003629691,-0.0002669833
H,0,-0.3414208815,0.9990588008,-0.0001013177
C,0,-3.7474654975,1.0104537536,-0.0002867714
H,0,-4.9839476288,-0.7543050307,-0.0001715542
H,0,-2.2611481024,2.5724976156,-0.0003676632
H,0,-4.5876636993,1.6992747354,-0.0004022025
N,0,0.7538350507,-1.3426252327,0.0001982029
O,0,1.6114396237,-2.4193288734,0.0003713998
C,0,3.0016746615,-1.9985485168,0.0003916014
C,0,3.2965966853,-1.1944794498,-1.2641205739
C,0,3.2964622828,-1.1941460031,1.2647235086
C,0,3.7549399411,-3.3251489428,0.0006085384
H,0,3.0608618975,-1.7841387527,-2.155359701
H,0,2.6975438405,-0.280950233,-1.2850299575
H,0,4.3550726203,-0.9181312479,-1.3023143245
H,0,3.0606007356,-1.7835606567,2.156090895
H,0,4.3549417401,-0.9178188297,1.3029735265
H,0,2.6974341442,-0.2805936492,1.285317245
H,0,4.8340377316,-3.1460333181,0.0006257078
H,0,3.50088255,-3.9127194934,0.8877636767
H,0,3.5009520325,-3.9129683963,-0.8864016169

TS1 Path1 R = Me

E(smd) = -1737.36464412
G(298) = 0.717889
Edisp = -0.25766520

Ti,0,0.1761460727,0.5730622623,0.3146797616
N,0,1.0646429234,-0.8563114303,0.7669598036
C,0,2.3459337257,-2.4683669088,2.022800651
C,0,1.1706972491,2.8803999837,0.4948951834
C,0,1.3235613902,2.1623800798,1.710997614
C,0,0.0220445366,1.9477044286,2.252686164
C,0,-0.9251118943,2.5611316727,1.3754592749
C,0,-0.2144109681,3.1275573238,0.2906748165
N,0,-1.498688435,0.4270584266,-1.1024989761
N,0,-1.655343331,-0.3950154519,0.9220144639
C,0,-2.2460577185,-0.288282067,-0.2655109121
C,0,-1.9185058394,1.0812914373,-2.3416720987
C,0,-1.8879222859,-1.4249650265,1.9350371534
H,0,-1.04318512,-1.2982521822,2.6208607814
H,0,-1.175468475,1.8732953902,-2.4826815001
C,0,1.7757338124,-0.428111832,-1.647991245
O,0,1.2763603166,0.7264851935,-1.6007357146
C,0,-0.7506428711,3.9966997374,-0.8043951428
H,0,-0.5683234231,5.0565457418,-0.5783345513
H,0,-0.2647504159,3.7903683493,-1.7635127753
H,0,-1.8267157592,3.8770049634,-0.9438471452
C,0,2.2553590415,3.4760840334,-0.3480931419
H,0,2.195472825,4.5720986353,-0.328020338
H,0,3.2482478859,3.2079663667,0.0225186244
H,0,2.1814043803,3.16557701,-1.3957447052
C,0,2.6242401766,1.8726311969,2.3942786958
H,0,2.964763125,2.7446319499,2.9693826254
H,0,2.5363083974,1.0375971409,3.0930742674
H,0,3.4150125803,1.6213591402,1.6814197724
C,0,-0.306430648,1.4158783952,3.6143582034

H,0,-0.4321007817,2.2377876164,4.3331730573
H,0,-1.237598638,0.8435520291,3.6108171005
H,0,0.4808859547,0.767212878,4.0063485661
C,0,-2.3914147618,2.6796573151,1.6450719953
H,0,-2.5765263063,3.2517826062,2.5633171563
H,0,-2.9088286053,3.1950525301,0.8318697177
H,0,-2.851538332,1.6940426571,1.7685307592
C,0,-3.1638187151,-1.2240840149,2.7656272732
H,0,-3.2435708071,-0.1973698531,3.1365526061
H,0,-4.0643609029,-1.4495043669,2.1883016765
H,0,-3.1489880919,-1.8939834338,3.6331557105
C,0,-1.8082971895,-2.8612888767,1.4038317984
H,0,-2.6596418197,-3.1018622561,0.7606298563
H,0,-0.8806057738,-3.0076449886,0.8460708169
H,0,-1.8191792094,-3.5694629388,2.2412206633
C,0,-1.8272144283,0.1949829964,-3.5923067735
H,0,-2.5440841347,-0.6306810851,-3.5541004613
H,0,-2.0539930914,0.790944203,-4.4840430695
H,0,-0.8226221802,-0.2148041866,-3.7152381847
C,0,-3.2939928149,1.76009945,-2.2856296407
H,0,-3.422820414,2.320631145,-1.3555386534
H,0,-3.3948739421,2.4608413687,-3.1221063864
H,0,-4.1113871922,1.0381017734,-2.3581030057
C,0,-3.5636590951,-0.9139666606,-0.6247240381
C,0,-4.7607854252,-0.4278993624,-0.084782648
C,0,-3.6173555367,-1.9906392219,-1.5184763576
C,0,-5.9822408197,-0.9985561947,-0.4371347267
H,0,-4.7320863988,0.4117424204,0.6031198094
C,0,-4.8374625117,-2.5706516037,-1.8612984667
H,0,-2.6944807476,-2.3846506782,-1.9339515959
C,0,-6.0240586739,-2.0731931098,-1.3246887577
H,0,-6.9028193287,-0.6028910894,-0.0165995038
H,0,-4.8601047264,-3.411741799,-2.5489804711
H,0,-6.9761649333,-2.5209012067,-1.5958242582
O,0,1.4289105271,-2.1494543567,0.9246225132
C,0,1.680917389,-2.1264228814,3.3510919138
H,0,1.4296178311,-1.0641352824,3.3796049616
H,0,0.7610087086,-2.703539897,3.482648215
H,0,2.3520481375,-2.3497149137,4.1866676405
C,0,3.6646238184,-1.7271278083,1.8458254956
H,0,4.3279083424,-1.9251803269,2.6942833938
H,0,4.1694891922,-2.0426852352,0.9297676608
H,0,3.4862836619,-0.6526735005,1.7862088682
C,0,2.5316943267,-3.9745203307,1.8741750104
H,0,2.9672037048,-4.2142002598,0.8995796328
H,0,3.2022283683,-4.3502726437,2.6529817578
H,0,1.5722746111,-4.4925273623,1.9629130016
C,0,3.2529939714,-0.6026048919,-1.5828784492
C,0,3.8579088406,-1.8478837253,-1.8118752184
C,0,4.070085749,0.5138284389,-1.3611991518
C,0,5.2451374477,-1.9710071267,-1.8113780177
H,0,3.2492433005,-2.7261182579,-1.9950593408
C,0,5.4539371706,0.3903995684,-1.3534444037
H,0,3.5937147039,1.472605629,-1.2036545972
C,0,6.0461214758,-0.8538615972,-1.5786667347
H,0,5.7007898896,-2.9402509196,-1.9933968195
H,0,6.0749197202,1.2647917032,-1.1791518966
H,0,7.1284310043,-0.9507897993,-1.5777479657
C,0,0.9544053478,-1.6200798679,-2.0616620767
H,0,-0.1016631263,-1.3662756411,-1.9964917735
H,0,1.2064204036,-1.8881699474,-3.0963817485
H,0,1.1655473722,-2.4776002984,-1.418111355

TS1 Path2 R = Me

E(smd) = -1737.36238833
G(298) = 0.714464
Edisp = -0.25755959

Ti,0,-0.4502482271,-0.9397588656,-0.069201679
N,0,-1.5453178032,0.1997105095,0.6469397399
C,0,-3.1601649114,1.2881701308,2.0665102353
C,0,-1.2664224777,-3.1670468054,-0.952423812
C,0,-1.7005191685,-2.9507543527,0.3833103121

C,0,-0.5436140582,-2.9385772542,1.2163295115
C,0,0.5968737465,-3.1798071624,0.3895987599
C,0,0.1492114525,-3.3073169275,-0.9462518863
N,0,1.4488500482,-0.2509291754,-0.9311864525
N,0,1.1192466043,-0.2468758083,1.2356307613
C,0,1.9473070117,0.0981150996,0.2525735473
C,0,2.1637869121,-0.3911168249,-2.2003441271
C,0,1.0657505296,0.321288707,2.5828766113
H,0,0.1283109022,-0.0741096563,2.988191205
H,0,1.5330778822,-1.0725687555,-2.7814409633
C,0,-2.0564704301,0.4053309053,-2.009648756
O,0,-1.0586867756,-0.3370402603,-2.1396162714
C,0,0.9526563432,-3.6909715308,-2.1506062265
H,0,0.8337478477,-4.7607918177,-2.3723476256
H,0,0.6321373688,-3.1458881673,-3.0444267178
H,0,2.0201015757,-3.5059252851,-2.0151478313
C,0,-2.1183111737,-3.4241174777,-2.1587779969
H,0,-1.9339069748,-4.4354800968,-2.5433487805
H,0,-3.1857062017,-3.3689066169,-1.9262659804
H,0,-1.9081301782,-2.7234163503,-2.9739725629
C,0,-3.1192863921,-2.9521973003,0.8646343608
H,0,-3.4540983375,-3.9740579623,1.0898228887
H,0,-3.2356923402,-2.3635734765,1.7775118856
H,0,-3.8104840274,-2.5421746574,0.1224899161
C,0,-0.52740988,-2.9355853083,2.714680079
H,0,-0.6117196683,-3.9571624367,3.1116982148
H,0,0.4013167151,-2.5115644209,3.1039524899
H,0,-1.3542124771,-2.3579222384,3.1357845861
C,0,1.992848436,-3.3727841079,0.8910160454
H,0,2.6830641442,-3.6104576578,0.077516704
H,0,2.3585222167,-2.4732918872,1.3972203614
H,0,2.040461279,-4.2003789052,1.6099033717
C,0,2.1823541175,-0.1558406171,3.5227678111
H,0,2.298332861,-1.2435888895,3.4853988904
H,0,3.1454570186,0.2985466296,3.2763876246
H,0,1.9389582173,0.1203800894,4.5552945379
C,0,0.9452979858,1.8500268524,2.6117636755
H,0,1.8739691506,2.3336817411,2.2946170012
H,0,0.1287611936,2.1766156277,1.9637929815
H,0,0.7319429859,2.1890920601,3.6328797557
C,0,2.2506729262,0.90083154,-3.024590406
H,0,2.8692513574,1.6540257263,-2.5272329017
H,0,2.7066514057,0.6874560283,-3.9985411947
H,0,1.2593313556,1.3206059607,-3.20615211
C,0,3.55050825,-1.0411578458,-2.0998353565
H,0,3.5358196224,-1.90806386,-1.4334328018
H,0,3.8717931658,-1.3795064257,-3.0914258514
H,0,4.3053819422,-0.3437249957,-1.7279838723
C,0,3.257989985,0.8070616889,0.4464131882
C,0,4.3584239959,0.1441480433,1.0039930197
C,0,3.4070012141,2.1433119245,0.0559091697
C,0,5.5787851406,0.7983786325,1.1590962498
H,0,4.2584400902,-0.894759381,1.3034428534
C,0,4.6236156749,2.8028210984,0.2218457029
H,0,2.5573408978,2.6708100819,-0.3670342607
C,0,5.714590551,2.1306244623,0.7704481635
H,0,6.4248458235,0.2658903052,1.5851409002
H,0,4.7187604336,3.8428692833,-0.0784177767
H,0,6.6650358227,2.6420126299,0.8952815777
O,0,-2.038728756,1.3616657749,1.1340704251
C,0,-2.7740078896,0.4599000592,3.2859712435
H,0,-2.4987181974,-0.5514811722,2.9797806576
H,0,-1.919545937,0.9095547694,3.7994816455
H,0,-3.6093666233,0.3980076167,3.9908109934
C,0,-4.3886012718,0.7152202454,1.3664424327
H,0,-5.2257297901,0.6281846697,2.0667926555
H,0,-4.6993394718,1.3703007928,0.546355833
H,0,-4.1683682324,-0.2771806656,0.9666953984
C,0,-3.3782086932,2.7508370414,2.4403107667
H,0,-3.5896320284,3.3457620547,1.5470448142
H,0,-4.2225197621,2.8443780546,3.1303934373
H,0,-2.487084714,3.1609984258,2.9237862409
C,0,-1.9204156787,1.8835806016,-2.0085548102
C,0,-2.9984927505,2.7148278351,-2.3478480675
C,0,-0.6869305815,2.4641775749,-1.6828576432
C,0,-2.8392842484,4.0971483425,-2.3840992666

H,0,-3.9621371339,2.2869502661,-2.6053765571
C,0,-0.5347286506,3.8448842371,-1.7050645278
H,0,0.1289004917,1.8095117313,-1.3929636328
C,0,-1.6073863023,4.6642436121,-2.0610309456
H,0,-3.6761525965,4.7309355242,-2.663318675
H,0,0.4211305222,4.288970112,-1.4419613932
H,0,-1.4841792124,5.7437549952,-2.0827070756
C,0,-3.4435344565,-0.177095306,-2.0834651844
H,0,-4.1475345938,0.3456448427,-1.4362501315
H,0,-3.8015004203,-0.0899734162,-3.1182196123
H,0,-3.4114727193,-1.2310948126,-1.8230105098

Intermediate Path1 R = Me (25b_int_Me_{down})

E(smd) = -1737.39158411
G(298) = 0.717534
Edisp = -0.25846405

Ti,0,-0.8899840471,-0.7517098235,-0.444887941
N,0,-1.7496144074,0.7071922342,0.5552035859
C,0,-2.7331470055,1.1846960212,2.7311493129
C,0,-2.2969210707,-2.1003154999,-1.8997201306
C,0,-2.6740607623,-2.2956808853,-0.5353844082
C,0,-1.6050997183,-2.9824566651,0.1103135642
C,0,-0.574285002,-3.1996557002,-0.8492761865
C,0,-1.0119075353,-2.6665546064,-2.0901869578
N,0,1.1031240559,-0.5351326519,-1.1023562539
N,0,0.691139281,-0.9610723786,1.0110596151
C,0,1.6229409729,-0.62460364,0.1203038282
C,0,1.7641770277,-0.2455521048,-2.3740603942
C,0,0.8404844485,-1.02374471,2.465327802
H,0,-0.1618930556,-1.2868453749,2.8152634708
H,0,0.9902416174,-0.4523972125,-3.11982448
C,0,-1.6789046237,1.6215972709,-0.5991382417
O,0,-1.418637391,0.6450344859,-1.5985514345
C,0,-0.3344911387,-2.78577842,-3.4198125914
H,0,-0.7188219747,-3.6580926458,-3.9654198946
H,0,-0.5211100629,-1.9102006077,-4.0487375722
H,0,0.7462387861,-2.9093982466,-3.3288138132
C,0,-3.1438975431,-1.5369113377,-2.996644706
H,0,-3.3467982552,-2.3026227237,-3.7557915936
H,0,-4.1084682553,-1.1898049457,-2.6203325115
H,0,-2.6524683043,-0.6936015831,-3.4927800104
C,0,-4.0305069869,-2.0090358192,0.0336884188
H,0,-4.7303482697,-2.8177477609,-0.2158252122
H,0,-4.0091718806,-1.922919114,1.1222492717
H,0,-4.4452946635,-1.0775095506,-0.359504281
C,0,-1.613329969,-3.5550756743,1.4943767877
H,0,-1.9032731505,-4.6141322402,1.4644701832
H,0,-0.6278166851,-3.5013852885,1.962692206
H,0,-2.3252652989,-3.0493318442,2.150675876
C,0,0.6907252623,-3.9573327655,-0.5962534276
H,0,0.475275084,-4.9726760011,-0.2412562192
H,0,1.289869968,-4.0505794389,-1.5050679713
H,0,1.3059816445,-3.4676372589,0.1660005647
C,0,1.7752000193,-2.1383280616,2.9571113266
H,0,1.5402420408,-3.0980750149,2.4864126204
H,0,2.8245039561,-1.9078695846,2.7576724713
H,0,1.6628336562,-2.2598903729,4.0404562212
C,0,1.1951708588,0.3150687968,3.1226612276
H,0,2.2298667462,0.6033702177,2.9190873978
H,0,0.5218199443,1.0957134129,2.7626577756
H,0,1.0848873498,0.2342099445,4.2107686965
C,0,2.154703104,1.2236273641,-2.5712601237
H,0,2.9326078435,1.5332114355,-1.8676834861
H,0,2.5475141286,1.3644915101,-3.584699609
H,0,1.2869339764,1.8735961388,-2.4525880039
C,0,2.9517969603,-1.1638692174,-2.694271402
H,0,2.7193541392,-2.2102468153,-2.4758211863
H,0,3.1984466847,-1.0853917664,-3.7588452719
H,0,3.8445395205,-0.89066289,-2.1265124829
C,0,3.0663688674,-0.3542187504,0.4384357836
C,0,3.9936660905,-1.4007424765,0.505422348
C,0,3.5084428612,0.9565899132,0.6529076059

C,0,5.3351676463,-1.1416269732,0.7798276008
H,0,3.6629397441,-2.4205958292,0.3329504202
C,0,4.8499523578,1.2149029662,0.929733299
H,0,2.796214483,1.7754193353,0.6115112103
C,0,5.7668035274,0.1668811228,0.9928209191
H,0,6.0435619011,-1.9641820656,0.8258928098
H,0,5.177081603,2.2374180134,1.0965641996
H,0,6.8125924652,0.3685744962,1.2069099261
O,0,-1.6389195809,1.3735010232,1.7882125319
C,0,-2.6058440177,-0.1850949029,3.396217353
H,0,-2.6260711137,-0.9722011063,2.6384338342
H,0,-1.67013946,-0.2620323126,3.9563350334
H,0,-3.4345085913,-0.359865259,4.0905731408
C,0,-4.1083785949,1.3347347055,2.0904188741
H,0,-4.8820059806,1.1269740272,2.8371375876
H,0,-4.2637979413,2.3430891876,1.7042826574
H,0,-4.2258246984,0.6334891992,1.2626742727
C,0,-2.4870183512,2.2950262666,3.7511225046
H,0,-2.5890033459,3.277574612,3.2815637073
H,0,-3.2109172966,2.2258259485,4.5692530322
H,0,-1.4809800432,2.2159862598,4.1738107374
C,0,-2.9734160216,2.3833794845,-0.905365401
C,0,-3.2691750169,3.6004117103,-0.2763017747
C,0,-3.8859316374,1.8877436788,-1.8394966754
C,0,-4.4492925084,4.2865938722,-0.5588362686
H,0,-2.5778646833,4.0193218371,0.4479462667
C,0,-5.0676728128,2.5703098988,-2.1245780136
H,0,-3.6420866404,0.9699408916,-2.3577220124
C,0,-5.3575699994,3.7728201425,-1.4831688815
H,0,-4.6561034681,5.228705377,-0.0571783111
H,0,-5.758668859,2.1656476673,-2.8602532031
H,0,-6.2752883369,4.3097707397,-1.7079351783
C,0,-0.5070877587,2.5996803922,-0.4771956621
H,0,0.4184479091,2.029958456,-0.3798698466
H,0,-0.4487481954,3.2362304437,-1.3647502744
H,0,-0.6129709719,3.2310453675,0.4073807213

Intermediate Path2 R = Me (25b_int_Me$_{up}$)

E(smd) = -1737.39273230
G(298) = 0.720173
Edisp = -0.26006199

Ti,0,-0.7001868174,-0.8950086692,-0.4012244384
N,0,-1.8332507645,0.4493810673,0.4363556022
C,0,-2.9770656646,0.7064293696,2.5954350499
C,0,-1.860405705,-2.6543359073,-1.6090619018
C,0,-1.9786376573,-2.9144624831,-0.2121812433
C,0,-0.6770889483,-3.2173342989,0.2814448896
C,0,0.2411009441,-3.1360206147,-0.8062691369
C,0,-0.4958110529,-2.7922665752,-1.9727653224
N,0,1.1127663976,-0.1072231749,-1.0750962931
N,0,0.8988926239,-0.6105877542,1.0529921089
C,0,1.6630614791,-0.0230869252,0.1353753364
C,0,1.5990277112,0.4242437412,-2.3482163786
C,0,1.1289667434,-0.637719374,2.4963210684
H,0,0.3076826685,-1.2513830254,2.8799899748
H,0,0.7707474833,0.2242868337,-3.0364883495
C,0,-2.2152111227,1.0745814785,-0.8326010111
O,0,-1.6228151519,0.1139801787,-1.7017511435
C,0,0.0013723428,-2.6727852116,-3.3803078689
H,0,-0.4037749879,-3.4846976041,-3.9980120987
H,0,-0.3129914263,-1.7317329824,-3.8435756796
H,0,1.0893732366,-2.7300044259,-3.4407326306
C,0,-2.9714799968,-2.3886921196,-2.5734492549
H,0,-3.0229757483,-3.1841640479,-3.3272987551
H,0,-3.9414535969,-2.3495649161,-2.0716891916
H,0,-2.821815378,-1.434602537,-3.0880964371
C,0,-3.2748440311,-3.0813407181,0.5230237406
H,0,-3.7071998172,-4.0681433887,0.3108992904
H,0,-3.1500618562,-3.0128810763,1.6058736497
H,0,-4.0137780891,-2.3321929106,0.2271395221
C,0,-0.3438881743,-3.7293941522,1.6484123727
H,0,-0.4064105047,-4.8258702526,1.6707091395

H,0,0.6707046576,-3.4542732894,1.9436891157
H,0,-1.0290695187,-3.3557583739,2.4144977733
C,0,1.6979527323,-3.4655371628,-0.7165745209
H,0,1.8449612989,-4.510029483,-0.4146669304
H,0,2.2016093501,-3.328933539,-1.6756603604
H,0,2.2049462812,-2.8352658621,0.0216669949
C,0,2.4235251838,-1.341133591,2.9292319807
H,0,2.5412954089,-2.3078159918,2.4296069757
H,0,3.3088821334,-0.7383314594,2.7149868274
H,0,2.3978153956,-1.5218403353,4.0097939426
C,0,1.0062455311,0.7346259794,3.1716567623
H,0,1.8780755761,1.3603867312,2.9639227289
H,0,0.1092673794,1.2506064896,2.8202447301
H,0,0.9406773971,0.6130870801,4.2597611156
C,0,1.8335226617,1.938631507,-2.3817218133
H,0,2.7508644157,2.2207735028,-1.8590079774
H,0,1.9340679699,2.2631331569,-3.4234628581
H,0,0.9943170303,2.478469127,-1.9411087184
C,0,2.8349958498,-0.3123701221,-2.8807572432
H,0,2.7008925169,-1.3961008533,-2.8530012694
H,0,3.0236427733,-0.0193479969,-3.9196407337
H,0,3.7265698031,-0.0634448409,-2.2984674541
C,0,2.9730825338,0.6597937297,0.4088007682
C,0,4.1769847254,-0.0487539333,0.3190134702
C,0,3.0086735564,2.0190465468,0.7421427735
C,0,5.3927619855,0.587083265,0.5659629188
H,0,4.1600936518,-1.1030718439,0.0582066106
C,0,4.2248163709,2.6533154721,0.9888166709
H,0,2.0807713339,2.5809416067,0.7893456019
C,0,5.4193282423,1.9392606567,0.90354765
H,0,6.319180869,0.0238818625,0.4940868996
H,0,4.2378473266,3.7094090068,1.2438236613
H,0,6.3666729925,2.435118351,1.0959369647
O,0,-2.0547585991,1.2165386983,1.5927469506
C,0,-2.4116586716,-0.5526051585,3.2470160981
H,0,-2.1907340972,-1.3016797554,2.4833443873
H,0,-1.4936648338,-0.3291484121,3.7945116279
H,0,-3.1332671033,-0.9828088651,3.9494636263
C,0,-4.3698627196,0.4411228334,2.0348150945
H,0,-5.0262671496,0.0797387623,2.8331331324
H,0,-4.8087663362,1.3524364823,1.6216674846
H,0,-4.3350988652,-0.3183455234,1.2525881112
C,0,-3.0236435624,1.8563132055,3.6010476049
H,0,-3.4151689929,2.7625842131,3.1301717567
H,0,-3.6711050923,1.5939762321,4.4434603416
H,0,-2.0239945303,2.071777514,3.9890239239
C,0,-1.6316822693,2.4658969002,-1.1195377405
C,0,-1.6935023691,2.9349819146,-2.4397809368
C,0,-1.0648692381,3.2966574508,-0.1478308077
C,0,-1.2139370617,4.1964223384,-2.7796741195
H,0,-2.1017662631,2.2896080423,-3.2122547634
C,0,-0.5828362944,4.5631003117,-0.48887329
H,0,-1.013668895,2.957198818,0.8788785305
C,0,-0.6575429221,5.0211259636,-1.8014802379
H,0,-1.2691560755,4.5342791045,-3.8114470407
H,0,-0.1509408266,5.1954476604,0.2832912933
H,0,-0.2843353541,6.0079210677,-2.0623452471
C,0,-3.7238061767,1.1047562244,-1.1047950919
H,0,-4.2264606588,1.8239737724,-0.4539749971
H,0,-3.9042239815,1.4027999437,-2.1410328943
H,0,-4.1469431954,0.1096668639,-0.9509680749

TS2 Path1 R = Me

E(smd) = -1737.37439946
G(298) = 0.718011
Edisp = -0.25825473

Ti,0,-0.2591135612,-0.6443823416,0.2987563896
N,0,-1.5917932598,1.2115818076,-0.0360977236
C,0,-1.6051907152,3.5887075884,0.2615890526
C,0,-1.8221006336,-1.0916458776,2.1273000773
C,0,-0.5716045634,-0.8847430852,2.7825362522
C,0,0.3155961373,-1.9009031895,2.3575108205

C,0,-0.3887554592,-2.7393731551,1.4346076326
C,0,-1.7144044415,-2.2507228108,1.3073079747
N,0,1.6373722617,-1.3684703064,-0.3959372782
N,0,1.4641814241,0.619131087,0.5135170422
C,0,2.2509789279,-0.2111815663,-0.1703304764
C,0,1.9260126003,-2.3261470803,-1.4670773102
C,0,1.8779166151,1.8406356193,1.2038564898
H,0,0.945075289,2.2306957091,1.6212389052
H,0,1.0912549483,-3.0319605245,-1.4112337803
C,0,-1.8558006384,0.697288683,-1.2659437049
O,0,-0.8538257376,-0.9475150439,-1.2740694519
C,0,-2.8165010474,-2.9214931053,0.5469820129
H,0,-3.6313907976,-2.2330009949,0.3139565955
H,0,-2.456168435,-3.327093113,-0.4022550651
H,0,-3.2371744511,-3.7529528686,1.1282097923
C,0,-3.0798693044,-0.3593620215,2.4698551056
H,0,-3.4799815086,-0.7313604858,3.4233774364
H,0,-2.9071705065,0.7127974304,2.5796053562
H,0,-3.8524420305,-0.5017322289,1.7132675331
C,0,-0.3261828241,0.181805577,3.8063846509
H,0,-1.0553101866,0.108356332,4.6227218089
H,0,0.6678501995,0.0958238558,4.2507668319
H,0,-0.4151566516,1.1907231987,3.3888910593
C,0,1.7179421876,-2.1477414424,2.8163972267
H,0,1.8053237214,-3.1345229569,3.2877040664
H,0,2.4157210875,-2.1228727489,1.9717439893
H,0,2.0448356794,-1.4057950121,3.5485424664
C,0,0.1180257217,-4.0348981456,0.8825967388
H,0,-0.116231905,-4.8585879796,1.57096849
H,0,-0.3437408031,-4.2792426104,-0.0782805898
H,0,1.2015423352,-4.0220118839,0.7465322562
C,0,2.8377070686,1.5755972375,2.3699609499
H,0,2.4484574778,0.8005253735,3.0332352591
H,0,3.8224960837,1.2596859225,2.0127327544
H,0,2.976394802,2.4897780333,2.9586194751
C,0,2.4370831618,2.9410320603,0.294154533
H,0,3.4510605716,2.7187943112,-0.0449127344
H,0,1.7920134698,3.080203947,-0.5757855793
H,0,2.4764643876,3.8872783789,0.8453952797
C,0,1.8786724439,-1.7284277712,-2.8778134486
H,0,2.7424879624,-1.0883310395,-3.0779969413
H,0,1.8845375115,-2.5330935778,-3.6222832195
H,0,0.9604823233,-1.1500601823,-3.0018804488
C,0,3.2103568095,-3.1360145501,-1.2481760113
H,0,3.2564793771,-3.5403858526,-0.2319833847
H,0,3.2395871937,-3.9783299397,-1.9486432134
H,0,4.1066380408,-2.5330181746,-1.4146411308
C,0,3.6509259463,0.0930264763,-0.6252971928
C,0,4.7422508255,-0.4147308073,0.0896278313
C,0,3.8927239182,0.863227765,-1.769181744
C,0,6.0470154542,-0.1516418758,-0.3249030916
H,0,4.5665440266,-1.0204010349,0.9741196625
C,0,5.1964755562,1.116499053,-2.1901177589
H,0,3.0542990984,1.2684372547,-2.3275904802
C,0,6.277427604,0.6121728933,-1.4676779674
H,0,6.8831065353,-0.5486348657,0.2442779208
H,0,5.3674381092,1.7121047066,-3.0826654918
H,0,7.2938669481,0.8133596659,-1.7943459071
O,0,-0.828678686,2.4294656525,-0.133127674
C,0,-2.2017718425,3.4137299394,1.6576346622
H,0,-2.9670685983,2.6360934397,1.6644871129
H,0,-1.4227538814,3.1374905107,2.3743765892
H,0,-2.6580006904,4.3514789105,1.9918693553
C,0,-2.7041356196,3.9073903985,-0.7571388145
H,0,-3.2916713249,4.7679719041,-0.4196474629
H,0,-2.2715169566,4.1597993506,-1.7298729142
H,0,-3.3908173517,3.0677470756,-0.8861158189
C,0,-0.5810476017,4.7220378842,0.2697135817
H,0,-0.0839079565,4.8010530537,-0.7013140324
H,0,-1.0813803369,5.6731258835,0.4772736841
H,0,0.180379764,4.560111535,1.0362917585
C,0,-3.1957012474,0.0368490102,-1.4537642021
C,0,-3.4111917884,-0.9118603018,-2.4642668435
C,0,-4.2895365179,0.4661180789,-0.6955046477
C,0,-4.6839234401,-1.4185644983,-2.7003473512
H,0,-2.5642422535,-1.2757731883,-3.0353258539

C,0,-5.5672263467,-0.0459689296,-0.9290086675
H,0,-4.1260468457,1.2055070972,0.0799384809
C,0,-5.7690127283,-0.9888329104,-1.9327212642
H,0,-4.8307647058,-2.1589603731,-3.4822098379
H,0,-6.403693206,0.300455007,-0.3277689883
H,0,-6.7628741349,-1.3864944153,-2.1196213366
C,0,-1.2827005061,1.3188318758,-2.5151128358
H,0,-1.883015606,2.1890541546,-2.7963553229
H,0,-0.2554647109,1.6421949975,-2.3535652491
H,0,-1.3261812615,0.5978591406,-3.3316537008

TS2 Path2 R = Me

E(smd) = -1737.37134414
G(298) = 0.718970
Edisp = -0.26047519

Ti,0,0.3472351034,1.0894209582,-0.3598523554
N,0,2.2019342669,-0.0195015684,0.2677337094
C,0,3.220761709,-1.2543862724,2.0413074034
C,0,1.7662786239,3.064150557,0.0338941647
C,0,0.7606497759,3.1209186124,1.0492975978
C,0,-0.4926217172,3.2826589689,0.413756163
C,0,-0.2665581155,3.3136082068,-0.997959178
C,0,1.127812196,3.2045173206,-1.2317449728
N,0,-1.7113871329,0.6386790705,-0.7138933848
N,0,-0.7601216949,0.0453937535,1.1701243244
C,0,-1.8529029745,-0.053117411,0.4130260964
C,0,-2.414209465,0.4238706571,-1.9818247356
C,0,-0.6302826828,-0.3303100186,2.5793032485
H,0,0.4045457758,-0.0718650445,2.818941418
H,0,-1.9143182233,1.1109460241,-2.6717893866
C,0,2.2834195566,-0.5098141281,-1.007702585
O,0,0.742321577,0.289661929,-1.8220847032
C,0,1.7669365272,3.3334846164,-2.5822175212
H,0,2.8581412906,3.3445386908,-2.5174459536
H,0,1.4830517881,2.5084537892,-3.2444225139
H,0,1.4632868739,4.2710748024,-3.062716554
C,0,3.2402688138,3.0579469711,0.3067833695
H,0,3.4831658387,3.7719427142,1.1023404774
H,0,3.5921214237,2.0699789418,0.6189189307
H,0,3.8125948914,3.3555805839,-0.5768333569
C,0,1.0428078103,3.1104235645,2.5207149233
H,0,1.7182052415,3.9320454324,2.7918512325
H,0,0.1302224531,3.237219345,3.1075887567
H,0,1.5214975948,2.1824893934,2.8478371269
C,0,-1.8306409197,3.4902722241,1.0494099548
H,0,-2.2216850976,4.4877174355,0.8124187994
H,0,-2.5574474268,2.7575817704,0.6812984303
H,0,-1.7857813003,3.4074884027,2.1372579199
C,0,-1.2915477016,3.6491294062,-2.035694
H,0,-1.3464277664,4.7372241181,-2.1794383202
H,0,-1.0503054007,3.2075962957,-3.0067761879
H,0,-2.2877483349,3.3083539347,-1.7457481081
C,0,-1.5398566249,0.4734694453,3.5157907911
H,0,-1.4446588264,1.5461910428,3.3343180341
H,0,-2.5907690906,0.1953767368,3.3942527378
H,0,-1.2648828168,0.2805871077,4.5590719062
C,0,-0.7724802561,-1.8317703944,2.8562025425
H,0,-1.8069425861,-2.1701689704,2.7611821246
H,0,-0.143353736,-2.4096662122,2.1758610349
H,0,-0.4502602657,-2.046794807,3.8818198821
C,0,-2.2210968151,-0.9797923694,-2.5656340557
H,0,-2.7644416271,-1.7338625207,-1.9884913661
H,0,-1.1590850338,-1.2338988542,-2.5853974874
C,0,-3.8965751599,0.8179994241,-1.9570513975
H,0,-4.0395372212,1.8041364132,-1.5036682526
H,0,-4.2817542437,0.8586326887,-2.9820796183
H,0,-4.5034414056,0.0983645206,-1.4019148289
C,0,-3.0977429728,-0.8153222362,0.7726379535
C,0,-4.2085040717,-0.1310347892,1.2812831501
C,0,-3.184980181,-2.2001066716,0.5888467493
C,0,-5.3774619802,-0.8169515337,1.6056026074
H,0,-4.1548311841,0.9446124336,1.4210297522

C,0,-4.3573874052,-2.8847307992,0.9032098535
H,0,-2.3296509047,-2.7426374462,0.1980481233
C,0,-5.4560558111,-2.1955509604,1.4147043732
H,0,-6.2288450572,-0.2716311706,2.003529819
H,0,-4.4106265557,-3.959084652,0.7499118439
H,0,-6.3687211061,-2.730204214,1.6625919118
O,0,2.0285709225,-1.058342176,1.2374378101
C,0,3.4314383492,-0.0736380811,2.9893768676
H,0,3.5744785623,0.8512325704,2.4263953905
H,0,2.5697259656,0.049577188,3.6527849729
H,0,4.3178462067,-0.2340895089,3.6126430809
C,0,4.4650255611,-1.4736159813,1.1795640445
H,0,5.3128822346,-1.7418250838,1.8184921639
H,0,4.3056775057,-2.2853498498,0.4642795606
H,0,4.7307697206,-0.5661254928,0.6321123162
C,0,2.9003907142,-2.5245563106,2.8273811542
H,0,2.7291721037,-3.3632100996,2.1466431848
H,0,3.7339110932,-2.7765542001,3.4904720742
H,0,2.0055430806,-2.3871930235,3.4394299968
C,0,2.0553189177,-1.9577112537,-1.3259788836
C,0,2.9360658293,-2.6518057634,-2.1630891935
C,0,0.9447707054,-2.6414767012,-0.811050922
C,0,2.7259369923,-3.9976812335,-2.4654170536
H,0,3.8014241969,-2.1501956829,-2.5831661636
C,0,0.7308756338,-3.9795332767,-1.1181250574
H,0,0.251512653,-2.1063679965,-0.1725233163
C,0,1.6229951482,-4.6662050175,-1.944362955
H,0,3.4260962054,-4.5178399974,-3.11328298
H,0,-0.1358984009,-4.4938032508,-0.7114018312
H,0,1.454775041,-5.7133464318,-2.1809893952
C,0,3.252660429,0.2255378207,-1.8994945691
H,0,4.261160115,-0.1653796627,-1.7142722444
H,0,3.0015291709,0.1045901866,-2.9537664609
H,0,3.2576966309,1.281821519,-1.6455443026
H,0,-2.6043581563,-1.0114500481,-3.5921868924

Ph(CON^{t}Bu)Me anti (25b_*anti*)

E(smd) = -597.385304292
G(298) = 0.227810
Edisp = -0.05672213

C,0,0.484030006,1.1505967028,-0.0130422301
C,0,-0.3161895929,2.3988654818,-0.0131652756
C,0,-1.721726326,2.2956864857,-0.0132332534
C,0,0.2359273515,3.6959297873,-0.0132099922
C,0,-2.5360929368,3.4228600834,-0.0133446703
H,0,-2.1931447931,1.3193950388,-0.0132008296
C,0,-0.5831339012,4.8214130702,-0.0133174825
H,0,1.3083655105,3.8160717292,-0.0131601548
C,0,-1.970538544,4.6959973167,-0.0133873293
H,0,-3.6161523673,3.3035122221,-0.013397396
H,0,-0.1268556363,5.8078291469,-0.0133476292
H,0,-2.6035684984,5.5791751707,-0.0134733914
N,0,1.7660247788,0.9859238083,-0.0130349274
O,0,2.5282802151,2.1292980325,-0.0131687109
C,0,3.9471722654,1.805080931,-0.0131577581
C,0,4.2940931321,1.0224106964,1.2512294284
C,0,4.2940515935,1.022136439,-1.2773865751
C,0,4.611706024,3.177743642,-0.0133177481
H,0,4.0188440657,1.5948952106,2.1424369906
H,0,3.7562765461,0.071811929,1.269838783
H,0,5.3688593105,0.8181461423,1.2896346345
H,0,4.0187666811,1.5944242165,-2.1687092477
H,0,5.3688176664,0.8178702163,-1.3157855104
H,0,3.7562408339,0.0715299364,-1.2957698198
H,0,5.7002838509,3.0697969189,-0.0133238274
H,0,4.322090818,3.7473561578,-0.9015345613
H,0,4.3221210378,3.7475483215,0.8747857727
C,0,-0.2435460866,-0.1735706377,-0.012899531
H,0,-0.8807979722,-0.2843547092,0.871735742
H,0,-0.8807613742,-0.2845675116,-0.8975348519
H,0,0.4917887418,-0.9790185157,-0.012790668

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Ph(CON^tBu)Me syn (25b_*syn*)

E(smd) = -597.390633070
G(298) = 0.223637
Edisp = -0.05607579

C,0,0.4507913116,1.5754830386,-0.0047005741
C,0,1.5030358392,0.5302369219,-0.0013241054
C,0,2.8611016196,0.8790087085,-0.0057236759
C,0,1.168871663,-0.8354305291,0.0063656004
C,0,3.8526480585,-0.1012865155,-0.0025642818
H,0,3.1555338897,1.9236461522,-0.0116750939
C,0,2.1575212893,-1.8100895932,0.0095010164
H,0,0.1209295619,-1.1144125318,0.009813938
C,0,3.5070913962,-1.4493025289,0.0050533752
H,0,4.8983232699,0.1944202528,-0.0060920943
H,0,1.875780098,-2.8597612252,0.0154577929
H,0,4.2792427822,-2.2136556419,0.007518106
N,0,-0.7670531236,1.1544107613,-0.0001601593
O,0,-1.6993973921,2.1668330883,-0.0035880613
C,0,-3.0530449664,1.6398763793,0.0017528376
C,0,-3.2889202094,0.8092279117,-1.2579971947
C,0,-3.2840299657,0.8222957552,1.270922591
C,0,-3.9072271406,2.9038997066,-0.0031271805
H,0,-3.1009296333,1.4107365957,-2.1526786268
H,0,-2.6222245187,-0.0559431201,-1.2767300033
H,0,-4.3236477231,0.4535426188,-1.2916741011
H,0,-3.0925903384,1.4330137571,2.1586063258
H,0,-4.3186134262,0.4670013451,1.3122755599
H,0,-2.6172520742,-0.0426507634,1.296016161
H,0,-4.9692714682,2.6421110478,0.0002776241
H,0,-3.6981411077,3.5140550732,0.8806076612
H,0,-3.7015697465,3.5048861187,-0.8939213201
C,0,0.840496779,3.0269433437,-0.0129778713
H,0,1.4459506369,3.2693071026,0.8672433892
H,0,1.4426358946,3.2601228905,-0.8979396053
H,0,-0.0443746455,3.6606621694,-0.0146057292

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