Titanium alkoxyimido (Ti=N–OR) complexes: reductive N–O bond cleavage at the boundary between hydrazide and peroxide ligands

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Supporting Information

Electronic structure and bonding

The DFT structure for $Ti(NOMe)Cl_2(NHMe_2)_2$, a model for $Ti(NO^tBu)Cl_2(NHMe_2)_2$ (**1**), is shown in Fig. S1 along with representations of the HOMO and HOMO-1 (Ti–N π-bonding). As stated in the main text, although the NO^tBu groups in **1** – **3** are formally net dianionic ligands, the oxidation state of N_α is only -1 (compared to -3 or -2 in an imide or hydrazide ligand). A reviewer has asked us to comment further on this. The formal $Ti{\equiv}N_\alpha$ triple bond in **1** – **3** contains one σ and two π components. These three orbitals are predominantly ligand-based (*cf.* Fig. S1), in agreement with the electronegativity differences between Ti and N ($\chi_P(Ti) = 1.54$; $\chi_P(N) = 3.04$),[1] and contain six electrons. Four of these originate from the NO^tBu moiety and two from $TiCl_2(NHMe_2)_2$. Thus the NO^tBu moiety has formally gained two electrons compared to free NO^tBu and is best viewed as formally dianionic (like NR (imide) and NNR_2 (hydrazide) R = alkyl, aryl). With respect to the oxidation state of N_α in **1** – **3** a consideration of the electronegativity values of Ti and N (see above) and O ($\chi_P(O) = 3.44$) show that in an $Cl_2Ti{=}N\text{-}OR$ (R = hydrocarbyl) unit the oxidation states of the atoms must formally be Cl = -1, Ti = +4, O = -2, "R" = +1 and thus N = -1. In a system $Cl_2Ti{=}NR$ (imide) the N is therefore in a -3 oxidation state and in $Cl_2Ti{=}N\text{-}NR_2$ each N is in -2 oxidation state.

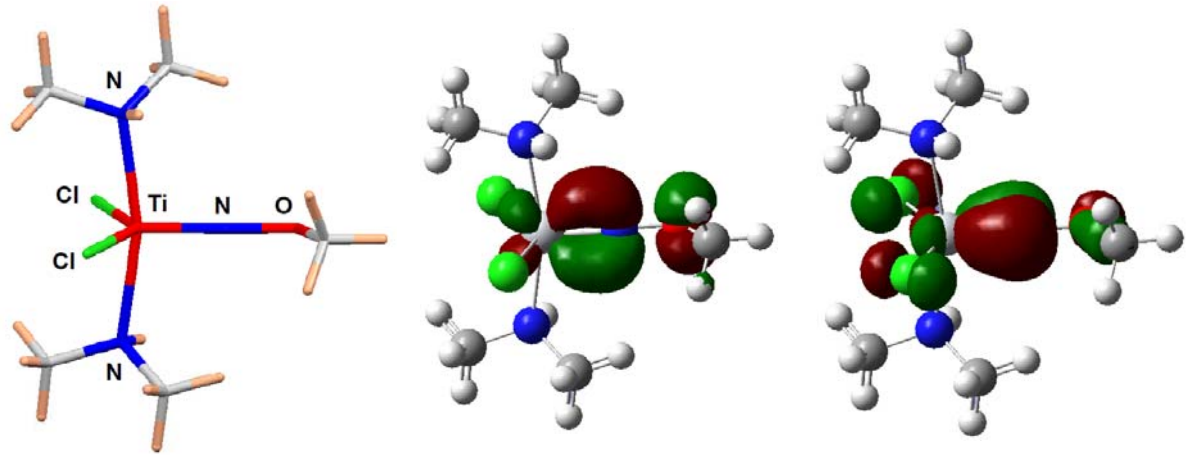


Figure S1. Left: minimized DFT structure for $Ti(NOMe)Cl_2(NHMe_2)_2$; centre: HOMO (-5.85 eV); right: HOMO-1 (-6.37 eV). Calculated distance (Å) and angles (°): Ti=NOMe 1.677, N–O 1.342, Ti–Cl 2.333 & 2.333, Ti–$NHMe_2$ 2.235 & 2.239 ; Ti=N–O 176.7, N–O–Me 111.5.

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 degassed by sparging with dinitrogen and dried by passing through a column of the appropriate drying agent.[2] Toluene was refluxed over sodium and distilled. Deuterated solvents were dried over sodium (C_6D_6) or P_2O_5 ($CDCl_3$ and CD_2Cl_2), distilled under reduced pressure and stored under dinitrogen 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 and ^{13}C-^{1}{H} NMR spectra were recorded on Varian Mercury-VX 300 and Varian Unity Plus 500 spectrometers at ambient temperature unless stated otherwise and referenced internally to residual protio-solvent (^{1}H) or solvent (^{13}C) resonances, and are reported relative to tetramethylsilane (δ = 0 ppm). Assignments were confirmed using two dimensional ^{1}H-^{1}H and ^{13}C-^{1}H NMR correlation experiments. Chemical shifts are quoted in δ (ppm) and coupling constants in Hz. IR spectra were recorded on a Nicolet Magna 560 E.S.P. FTIR spectrometer. Samples were prepared in a dry-box as Nujol mulls between NaCl plates or as a solution in dichloromethane, and the data are quoted in wavenumbers (cm^{-1}). Elemental analyses were carried out by Elemental Microanalysis Ltd.

Starting materials. ^{t}BuONH$_2$,[3] Ti(NMe$_2$)$_2$Cl$_2$,[4] Me$_3$TACH,[5] and Li$_2$N$_2$N^{Me},[6] were synthesised according to published procedures. Other reagents were purchased from Sigma-Aldrich and used without further purification.

Ti(NO^{t}Bu)Cl$_2$(NHMe$_2$)$_2$ (1). To Ti(NMe$_2$)$_2$Cl$_2$ (3.79 g, 18.4 mmol) in benzene (20 mL) cooled to 5 °C was added a solution of ^{t}BuONH$_2$ (2.00 mL, 18.4 mmol) in benzene (20 mL) dropwise. The dark brown mixture was then stirred for a further 4 h, after which time the slurry was filtered and washed with pentane (3 × 15 ml) to give **1** as a green solid. Yield: 1.45 g (51%). Diffraction-quality crystals were grown from a saturated toluene solution at RT. ^{1}H NMR (C_6D_6, 299.9 MHz): 2.84 (2H, br. m, N<u>H</u>Me$_2$), 2.33 (12H, d, ^{3}J = 6.0 Hz, NH<u>Me</u>$_2$), 1.19 (9H, s, ^{t}Bu). ^{13}C-{^{1}H} NMR (CD_2Cl_2, 75.4 MHz): 86.4 (O<u>C</u>Me$_3$), 41.0 (HN<u>Me</u>$_2$), 26.9 (OC<u>Me</u>$_3$). IR (NaCl plates, Nujol mull, cm^{-1}): 3247 (m, ν(N–H)), 1366 (s), 1261 (w), 1242 (w), 1157 (m) 1007 (m), 989 (m), 826 (m), 722 (m), 699 (w). IR (NaCl cell, CH_2Cl_2): 3289 (s, ν(N-H), cm^{-1}). EI-MS: [*M* - NMe$_2$]$^+$ 251 (20%). Anal. found (calcd. for $C_8H_{23}Cl_2N_3OTi$); C, 30.00 (32.45); H, 7.27 (7.83); N, 14.18 (14.19) %. The low %C found for carbon is attributed to incomplete combustion. The ^{1}H and ^{13}C-{^{1}H} NMR spectra of crystalline **1** are given below.

Ti(NO^{t}Bu)(Me$_3$TACH)Cl$_2$ (2). To a slurry of Ti(NO^{t}Bu)Cl$_2$(NHMe$_2$)$_2$ (**1**) (2.10 g, 3.40 mmol) in benzene (30 mL) cooled to 5 °C was added a solution of Me$_3$TACH (1.00 mL, 3.40 mmol) in benzene (20 ml) dropwise. The mixture was stirred for a further 16 h, after which time the slurry was concentrated (*ca*. 50%), filtered and washed with cold (0 °C) dichloromethane (3 × 15 ml) to give **2**

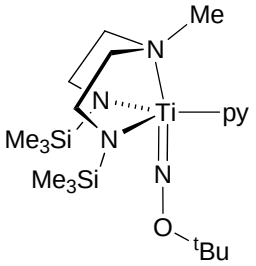
as a pink crystalline solid. Yield: 1.70 g (72%). Diffraction-quality crystals were grown from a saturated dichloromethane solution layered with hexanes. ^{1}H NMR (CD_2Cl_2, 299.9 MHz): 4.76 (1H, d, ^{2}J = 4.8 Hz, CH_2 *trans* to NO^{t}Bu), 4.26 (2H, d, ^{2}J = 4.5 Hz, CH_2 *trans* to Cl), 3.73 (1H, d, ^{2}J = 4.8 Hz, CH_2 *trans* to NO^{t}Bu), 3.36 (2H, d, ^{2}J = 4.5 Hz, CH_2 *trans* to Cl), 2.84 (6H, s, NMe *trans* to Cl), 2.16 (3H, s, NMe *trans* to NO^{t}Bu), 1.29 (9H, s, O^{t}Bu). ^{13}C-{^{1}H} NMR (CD_2Cl_2, 75.4 MHz): 86.0 ($\underline{C}Me_3$), 78.3 (CH_2 *trans* to Cl), 76.8 (CH_2 *trans* to NO^{t}Bu), 41.3 (NMe *trans* to Cl), 37.0 (NMe *trans* to NO^{t}Bu), 27.0 ($C\underline{Me}_3$). IR (NaCl plates, Nujol mull, cm^{-1}): 1364 (w), 1358 (w), 1261 (m), 1178 (m), 1158 (s), 1120 (w), 1083 (w), 1011 (m), 937 (m), 836 (m), 748 (m), 721 (w), 703(m). Anal. found (calcd. for $C_{10}H_{24}Cl_2N_4OTi$); C, 35.91 (35.84); H, 7.03 (7.22); N, 16.39 (16.72) %.

Ti(NO^{t}Bu)Cl$_2$(py)$_3$ (3). Ti(NO^{t}Bu)(Me$_3$TACH)Cl$_2$ (**2**) (1.00 g, 2.7 mmol) was dissoved in pyridine (10 ml) to form a dark purple solution. After 10 min hexanes (25 ml) were added and the resulting slurry filtered. The procedure was repeated and the product was dried *in vacuo* to yield **3** as a dark purple crystalline powder. Yield: 0.80 g (67%), Diffraction-quality crystals were grown from a saturated 1:1 (v/v) mixture of pyridine and hexanes at 4 °C. ^{1}H NMR (CD_2Cl_2, 299.9 MHz, 253 K): 9.04 (4H, d, ^{3}J = 5.4 Hz, 2-py *cis* to NO^{t}Bu), 8.63 (2H, br. m, 2-py *trans* to NO^{t}Bu), 7.82 (2H, t, ^{3}J = 7.2 Hz, 4-py *cis* to NO^{t}Bu) 7.71 (1H, br. m, 4-py *trans* to NO^{t}Bu), 7.36 (4H, app. t, ^{3}J = 7.2 Hz, 3-py *cis* to NO^{t}Bu), 7.19 (2H, br. m, 3-py *trans* to NO^{t}Bu), 1.13 (9H, s, O^{t}Bu). ^{13}C-{^{1}H} NMR (CD_2Cl_2, 75.4 MHz, 253 K): 151.7 (2-py *cis* to NO^{t}Bu), 151.0 (2-py *trans* to NO^{t}Bu), 138.6 (4-py *cis* to NO^{t}Bu), 137.4 (4-py *trans* to NO^{t}Bu), 124.0 (3-py *cis* to NO^{t}Bu), 123.4 (4-py *trans* to NO^{t}Bu), 86.0 (O$\underline{C}$Me$_3$), 26.8 (OC$\underline{Me}_3$). IR (NaCl plates, Nujol mull, cm^{-1}): 1603 (s), 1597 (s), 1364 (m), 1227 (m), 1150 (m), 1068 (w), 1039 (m), 1004 (w), 832 (w), 768 (s), 760 (s), 702 (s), 632 (w). Anal. found (calcd. for $C_{19}H_{24}Cl_2N_4OTi$); C, 51.62 (51.49); H, 5.46 (5.37); N, 12.64 (12.38) %.

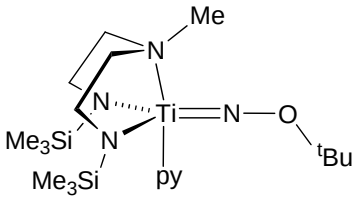
Alternative "one pot" synthesis of Ti(NO^{t}Bu)Cl$_2$(py)$_3$ (3). To a slurry of Ti(NMe$_2$)$_2$Cl$_2$ (5.00 g, 0.025 mol) in benzene (40 ml) at 5 °C was added dropwise a solution of $H_2NO^{t}Bu$ (3.35 mL, 0.025 mol) in benzene (12 mL). The resulting dark red solution was stirred for 14 h, after which time the solution was cooled to 5 °C and Me$_3$TACH (3.55 ml, 0.025 mol) was added dropwise. A precipitate immediately formed and the mixture was stirred for 14 h. The solid was filtered and washed with benzene (3 × 15 ml) at RT and dichloromethane (3 × 15 ml) at 0 °C. The light pink precipitate was dissolved in pyridine (10 ml), crystallised by addition of hexanes (50 ml) and filtered. This procedure was repeated twice. The product was then washed with pentane (3 × 15 ml) and dried i*n vacuo* to give **3** as a purple crystalline powder. Yield: 4.63 g (41%). The ^{1}H NMR spectrum was identical to that of a sample prepared from isolated **2** (see above).

Ti(N$_2$N^{Me})(NO^{t}Bu)(py) (4). A mixture of Ti(NO^{t}Bu)Cl$_2$(py)$_3$ (**3**) (1.00 g, 2.26 mmol) and $Li_2N_2N^{Me}$ (0.62 g, 2.26 mmol) was cooled to -78 °C and cold toluene (15 mL) was added. The mixture was allowed to warm to RT and was stirred for a further 60 min. The volitiles were removed under

reduced pressure and the solid residue extracted into diethyl ether (3 × 15ml). The volatiles were again removed to afford **4** as a green solid which was dried *in vacuo*. Yield: 0.92 g (86%). Diffraction-quality crystals were grown from a saturated hexanes solution at 4 °C. Compound **4** exists as a mixture of isomers designated **4a** (NO^{t}Bu *trans* to NMe) and **4b** (NO^{t}Bu *cis* to NMe) (ratio **4a**:**4b** = 3:1).



4a



4b

^{1}H NMR (C_6D_6, 299.9 MHz) for **4a**.: 8.40 (2H, br. d, ^3J = 4.5 Hz, 2-py) 6.73 (1H, m, overlapping 4-py), 6.45 (2H, m, overlapping 3-py), 3.63 (4H, overlapping 2 x m, CH_2), 2.61 (2H, m, CH_2), 1.98 (2H, m, CH_2), 1.15 (3H, s, NMe), 1.04 (9H, s, O^{t}Bu), 0.50 (18H, s, $SiMe_3$) ppm. ^{1}H NMR (C_6D_6, 299.9 MHz) for **4b**.: 8.71 (2H, br. d, ^3J = 5.4 Hz, 2-py), 6.73 (1H, m, overlapping 4-py), 6.45 (2H, m, overlapping 3-py), 3.40 (4H, 2 x overlapping m, CH_2), 2.81 (2H, m, CH_2), 2.45 (2H, m, CH_2), 1.41 (9H, br. s, O^{t}Bu), 0.16 (18H, s, $SiMe_3$) ppm. IR (NaCl plates, Nujol mull, cm^{-1}): 1357 (m), 1241 (m), 1190 (w), 1154 (w), 1092 (m), 1040 (m), 940 (s), 830 (s), 798 (m), 768 (m), 709 (w), 684 (w), 497 (s). Anal. found (calcd. for **4** - 0.5(py), $C_{17.5}H_{40.5}N_{4.5}OSi_2Ti$); C, 48.76 (48.42); H, 9.46 (9.40); N, 14.20 (14.52) %.

Ti{MeN(CH$_2$CH$_2$NSiMe$_3$)(CH$_2$CH$_2$NC(Me)C(Ph)NSiMe$_3$)(O^{t}Bu) (5). To a green solution of Ti(N_2N^{Me})(NO^{t}Bu)(py) (**4**) (0.20 g, 0.43 mmol) in benzene was added PhCCMe (54 µL, 0.43 mmol), immediately giving a colour change to dark red. After 1 h the volatiles were removed under reduced pressure and the resides. Crystallisation of the residues from a concentrated hexanes (10 mL) solution at 5 °C gave **5** as a dark red crystalline solid that was filtered and dried *in vacuo*. Yield 0.15 g (69%). Diffraction-quality crystals were grown from a saturated hexanes solution at 5 °C. ^{1}H NMR (C_6D_6, 299.9 MHz): 7.75 (2H, d, ^3J = 8.9 Hz, 2-Ph), 7.28 (2H, app. t, ^3J = 8.9 Hz, 3-Ph), 7.08 (1H, app. t, ^3J = 8.9 Hz, 4-Ph), 3.59 (3H, m, overlapping C$\underline{H}_2$C$\underline{H}_2$NMe), 3.36 (1H, m, C$\underline{H}_2$CH$_2$NMe), 2.82 (1H, m, C$\underline{H}_2$NMe), 2.58 (1H, m, C$\underline{H}_2$NMe), 2.34 (2H, m, C$\underline{H}_2$NMe), 2.16 (3H, s, NMe), 2.09 (3H, s, NCMe), 1.00 (9H, s, O^{t}Bu), 0.55 (9H, s, CH$_2$NSi$\underline{Me}_3$), 0.15 (9H, s, C(Ph)NSi$\underline{Me}_3$). ^{13}C-{^{1}H} NMR (C_6D_6, 75.4 MHz): 142.4 (1-Ph), 131.3 (2-Ph), 127.5 (3-Ph), 125.5 (4-Ph), 123.6 (C(Ph)NSiMe$_3$), 120.38 (N$\underline{C}$Me), 78.1 (O$\underline{C}$Me$_3$), 62.2 ($\underline{C}$H$_2$NMe), 61.2 ($\underline{C}$H$_2$NMe), 50.8 ($\underline{C}$H$_2$CH$_2$NMe), 50.6 ($\underline{C}$H$_2$CH$_2$NMe), 43.0 (NMe), 33.01 (OC$\underline{Me}_3$), 15.8 (NC$\underline{Me}$), 3.5 (C(Ph)NSi$\underline{Me}_3$), 1.4 (CH$_2$NSi$\underline{Me}_3$). EI-MS: $[M]^+$ 510 (100%). IR (NaCl plates, Nujol mull, cm^{-1}): 1455 (m), 1328 (m), 1237 (s), 1191 (m), 1101 (w), 1079 (w), 1067 (w), 1019 (s), 970 (w), 908 (m),

835 (s), 835 (m), 758 (w), 702 (w), 495 (s). Anal. found (calcd. for $C_{24}H_{46}N_4OSi_2Ti$); C, 56.51 (56.44); H, 9.03 (9.08); N, 10.88 (10.97) %.

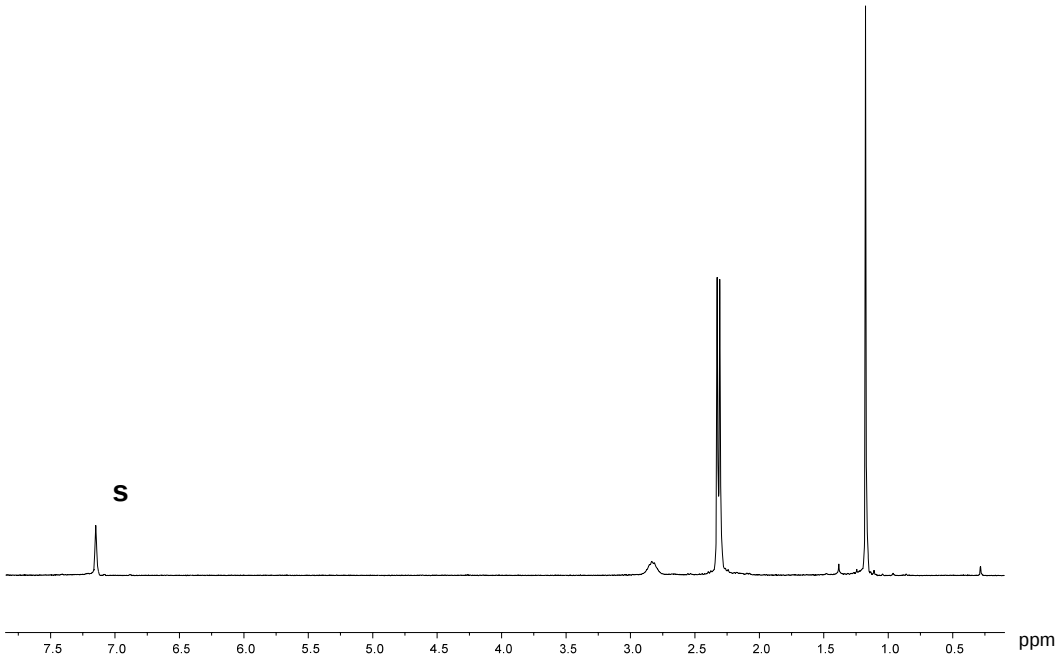


Figure S2. ^{1}H NMR spectrum (299.9 MHz, 298 K, C_6D_6) of $Ti(NO^tBu)Cl_2(NHMe_2)_2$ (**1**). "**s**" denotes residual protio-solvent.

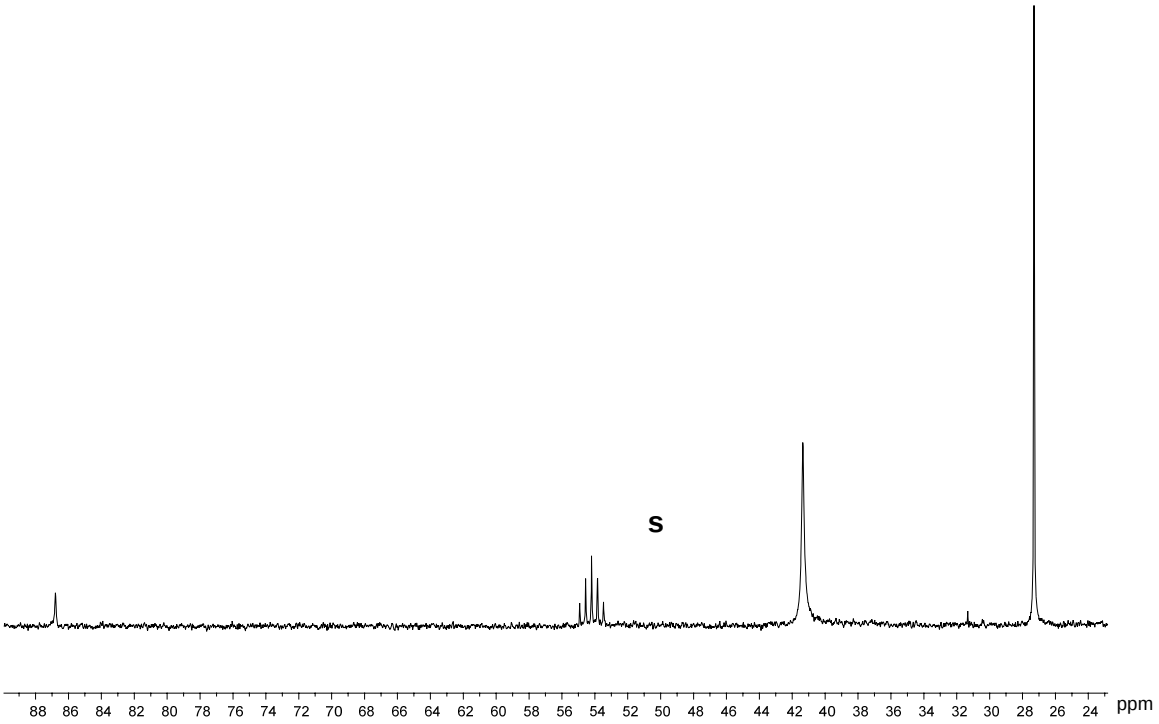


Figure S3. ^{13}C-{^{1}H} NMR spectrum (CD_2Cl_2, 75.4 MHz) of $Ti(NO^tBu)Cl_2(NHMe_2)_2$ (**1**). "**s**" denotes solvent resonance.

Computational details. All calculations were performed with the Gaussian03 package[7] of programs with the hybrid B3PW91 functional.[8, 9] The Ti atom was represented by the relativistic effective core potential (RECP) from the Stuttgart group and the associated basis set.[10] The remaining atoms (C, H, N, O) were represented by a 6-31G(*d*,*p*) basis set.[11] The Si atom was represented by RECP from the Stuttgart group and the associated basis set,[12] augmented by a *d* polarization function.[13] Full optimization of geometry was performed without any symmetry constraint, followed by analytical computation of the Hessian matrix to identify the nature of the located extrema as minima or transition states. Connection between reactant and product through a given transition state was checked by optimization of slightly altered geometries of the transition state along the two directions of the transition state vector associated to the imaginary frequency.

Crystal structure determinations of $Ti(NO^tBu)Cl_2(NHMe_2)_2$ (1), $Ti(NO^tBu)Cl_2(py)_3$ (3), $Ti(N_2N^{Me})(NO^tBu)(py)$ (4a), and $Ti\{MeN(CH_2CH_2NSiMe_3)(CH_2CH_2NC(Me)C(Ph)N\text{-}SiMe_3)(O^tBu)$ (5). Crystal data collection and processing parameters are given in Table S1. 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 an Enraf-Nonius KappaCCD diffractometer. As appropriate, absorption and decay corrections were applied to the data and equivalent reflections merged.[14] The structures were solved with SIR92[15] and further refinements and all other crystallographic calculations were performed using the CRYSTALS program suite.[16] 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.

Table S1. X-ray data collection and processing parameters for $Ti(NO^tBu)Cl_2(NHMe_2)_2$ (**1**), $Ti(NO^tBu)Cl_2(py)_3$ (**3**), $Ti(N_2N^{Me})(NO^tBu)(py)$ (**4a**), and $Ti\{MeN(CH_2CH_2NSiMe_3)(CH_2CH_2NC(Me)C(Ph)NSiMe_3)(O^tBu)$ (**5**).

Compound	**1**	**3**	**4a**	**5**
empirical formula	$C_8H_{23}Cl_2N_3OTi$	$C_{19}H_{24}Cl_2N_4OTi$	$C_{20}H_{43}N_5OSi_2Ti$	$C_{24}H_{46}N_4OSi_2Ti$
fw	296.10	443.23	473.67	510.73
temp / K	150	150	150	150
wavelength / Å	0.71073	0.71073	0.71073	0.71073
space group	$P\ \bar{1}$	$P\ 2_1/c$	$P\ 2_12_12_1$	$P\ 2_1/c$
a / Å	9.64230(10)	8.79620(10)	10.0550(2)	9.83180(10)
b / Å	11.1483(2)	21.8932(3)	15.5409(3)	17.1954(2)
c / Å	16.3073(3)	11.4868(2)	17.4207(4)	17.3784(2)
α / deg	107.0308(6)	90	90	90
β / deg	90.9663(7)	97.1358(6)	90	102.9629(7)
γ / deg	113.4410(7)	90	90	90
V / Å^3	1519.88(4)	2194.96(5)	2722.22(10)	2863.15(6)
Z	2	4	4	4
d (calcd) / Mg·m^{-3}	1.294	1.341	1.156	1.185
abs coeff / mm^{-1}	0.898	0.649	0.421	0.405
R indices:[a] R_1 =	0.0401[b]	0.0323[b]	0.0390[b]	0.0407[b]
R_w =	0.0407[b]	0.0307[b]	0.0457[b]	0.0412[b]

[a] $R_1 = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$; $R_w = \sqrt{\{\Sigma w (|F_o|-|F_c|)^2 / \Sigma w|F_o|^2\}}$; w$R2 = \sqrt{\{\Sigma w (F_o^2-F_c^2)^2 / \Sigma w(F_o^2)^2\}}$;

[b] For data wih $I > 3\sigma(I)$.

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Cartesian coordinates, electronic (E) and Gibbs free (G) energies in a.u.

MeCCMe
E: -155.922666617
G:-155.867008

C	0.605122	-0.000055	0.000103
C	-0.605109	-0.000296	0.000339
C	2.061951	0.000078	-0.000083
H	2.459864	1.020213	-0.043720
H	2.460264	-0.472271	0.904987
H	2.459847	-0.547618	-0.861842
C	-2.061976	0.000104	-0.000123
H	-2.459613	1.021230	-0.008834
H	-2.459753	-0.517701	-0.880211
H	-2.460533	-0.502840	0.888195

Pyridine
E: -248.191337776
G: -248.129579

C	1.140111	-0.720333	-0.000008
C	-1.139022	-0.722076	-0.000067
C	1.196331	0.672828	-0.000067
H	2.058855	-1.305495	0.000763
C	-1.197367	0.671101	0.000051
H	-2.056895	-1.308523	0.000118
C	-0.001044	1.383780	-0.000001
H	2.155132	1.182613	-0.000151
H	-2.156954	1.179402	0.000261
H	-0.001790	2.470476	0.000041
N	0.001086	-1.418609	-0.000068

I1a
E: -849.135439
G: -848.831479

Ti	0.149972	0.246304	0.255864
N	0.382983	0.442310	-1.430549
N	1.925844	-0.419496	0.768791
N	-1.594394	-0.674032	0.479725
N	-0.021590	-0.021228	2.648999
Si	3.154134	-0.537914	-0.475182
Si	-2.566132	-1.130459	-0.902525
C	2.217349	-0.884890	2.114402
C	0.903808	-1.155441	2.836401
C	-1.422411	-0.403779	2.896430
C	-1.949860	-1.272676	1.760704
C	0.370952	1.103311	3.500089
H	2.818276	-0.155462	2.685835
H	2.805063	-1.816014	2.123948

H	1.057549	-1.362478	3.909422
H	0.442145	-2.038894	2.385236
H	-1.536250	-0.901431	3.875160
H	-2.007104	0.522991	2.925162
H	-3.040482	-1.362224	1.889359
H	-1.562124	-2.300820	1.863962
H	-0.301437	1.947719	3.331807
H	0.335952	0.835048	4.568407
H	1.386895	1.422027	3.256335
C	-1.256238	2.975924	0.710809
C	1.029160	3.189827	0.434101
C	-1.421335	4.354266	0.774882
H	-2.098894	2.293765	0.776842
C	0.948480	4.575222	0.495766
H	1.973804	2.678633	0.274356
C	-0.298623	5.171991	0.669248
H	-2.414819	4.771339	0.902736
H	1.850938	5.169581	0.398935
H	-0.394166	6.252818	0.714647
N	-0.052986	2.398996	0.545488
H	3.515005	0.795673	-1.060701
H	2.800688	-1.460886	-1.596685
H	4.417805	-1.076316	0.155102
H	-2.785758	0.019814	-1.830722
H	-2.022895	-2.275605	-1.709248
H	-3.924542	-1.570544	-0.411276
O	0.773523	0.752340	-2.684672
C	-0.240476	0.491376	-3.647032
H	-0.525522	-0.566875	-3.632255
H	-1.127183	1.108707	-3.460757
H	0.195556	0.746894	-4.616155

I1a_full

E: -1202.93821174

G: -1202.390419

Ti	-0.069508	-0.432140	0.116157
N	0.056669	1.043239	-0.743092
N	-1.574693	-1.342462	-0.783379
N	1.777164	-1.182281	0.155012
N	-0.335658	-2.451955	1.414832
N	-0.616589	0.526578	2.021573
Si	-2.478087	-0.612073	-2.124930
Si	3.169563	-0.654740	-0.814839
O	0.057614	2.147199	-1.537078
C	0.361611	3.415676	-0.889812
C	0.401666	4.391839	-2.061274
C	-0.756477	3.778864	0.086518

C	1.710298	3.349051	-0.180850
C	-1.829256	-2.752579	-0.509166
C	-0.681224	-3.346907	0.297042
C	2.071308	-2.404591	0.904829
C	1.005398	-2.698013	1.953242
C	-1.342117	-2.538781	2.470954
C	-1.387381	-0.360783	-3.651711
C	-3.923387	-1.754961	-2.626236
C	-3.242963	1.045701	-1.619431
C	2.705511	0.218529	-2.421678
C	4.327515	0.435012	0.233967
C	4.200073	-2.177192	-1.335904
C	0.339296	0.879818	2.898028
C	0.055318	1.548238	4.083770
C	-1.268724	1.866963	4.374923
C	-2.259846	1.506288	3.464337
C	-1.892819	0.839105	2.301689
H	1.189567	4.111797	-2.766275
H	0.596359	5.408427	-1.705459
H	-0.553971	4.386191	-2.593787
H	-0.831006	3.026321	0.874946
H	-0.558691	4.750507	0.552038
H	-1.718152	3.834621	-0.432289
H	1.696272	2.567517	0.582885
H	1.935560	4.307225	0.299130
H	2.510143	3.120797	-0.890801
H	-2.780981	-2.901961	0.031361
H	-1.920560	-3.359023	-1.424158
H	-0.922155	-4.361289	0.661697
H	0.193375	-3.417583	-0.354885
H	3.031142	-2.342471	1.446980
H	2.177934	-3.280804	0.243355
H	1.131986	-2.017575	2.804885
H	1.107093	-3.729102	2.337806
H	-1.085059	-1.859033	3.287113
H	-2.322588	-2.255831	2.081477
H	-1.410820	-3.560654	2.879193
H	-0.565644	0.317167	-3.406392
H	-1.958294	0.068278	-4.483560
H	-0.962313	-1.312810	-3.988398
H	-4.593689	-1.965501	-1.785474
H	-4.517360	-1.265322	-3.406571
H	-3.580392	-2.712570	-3.032066
H	-3.879145	0.933764	-0.733790
H	-3.865077	1.446529	-2.428209
H	-2.451174	1.766218	-1.402983
H	2.123973	-0.460329	-3.054094
H	2.105324	1.116205	-2.265393

H	3.618518	0.487987	-2.966904
H	4.639525	-0.092740	1.142933
H	3.838721	1.366367	0.534973
H	5.235099	0.694908	-0.323195
H	5.029625	-1.853850	-1.975160
H	3.595708	-2.884340	-1.915613
H	4.631391	-2.718694	-0.487530
H	1.355363	0.616648	2.617275
H	0.862262	1.813045	4.758998
H	-1.523384	2.390804	5.291561
H	-3.304122	1.739245	3.644122
H	-2.623813	0.546286	1.554163

I1b

E: -849.133614

G: -848.831236

Ti	-0.293165	-0.012459	-0.263998
N	1.395381	-0.124813	-0.461551
N	-1.008034	1.851385	-0.416763
N	-1.283077	-1.770506	-0.277423
N	-1.225983	-0.016375	-2.346000
Si	-0.186093	3.240344	0.250245
Si	-0.817156	-3.168962	0.648999
C	-1.940572	2.172168	-1.488045
C	-2.386900	0.879754	-2.161181
C	-1.654320	-1.396419	-2.644379
C	-2.200890	-2.048339	-1.378168
C	-0.320815	0.495169	-3.384127
H	-1.490120	2.843018	-2.242272
H	-2.841223	2.696826	-1.127837
H	-2.892715	1.070361	-3.121933
H	-3.096867	0.364740	-1.506089
H	-2.379998	-1.415615	-3.475175
H	-0.760689	-1.946360	-2.955578
H	-2.314398	-3.125440	-1.586996
H	-3.222066	-1.688679	-1.167820
H	0.538764	-0.171824	-3.465653
H	-0.829753	0.561627	-4.359004
H	0.048823	1.481491	-3.100541
C	-1.382850	-0.025043	2.671833
C	0.917206	0.177115	2.628754
C	-1.410102	0.031168	4.059544
H	-2.292834	-0.138580	2.090618
C	0.977469	0.243044	4.016737
H	1.805552	0.229275	2.007821
C	-0.205639	0.168249	4.746076

H	-2.357265	-0.033140	4.584624
H	1.938751	0.349976	4.508229
H	-0.190705	0.214647	5.831299
N	-0.243413	0.045489	1.965831
H	0.803226	2.819792	1.285137
H	-1.149087	4.200899	0.901527
H	0.530077	4.035755	-0.809292
H	0.311709	-2.843574	1.571706
H	-1.940208	-3.714750	1.497242
H	-0.398391	-4.313538	-0.237786
O	2.750511	-0.114076	-0.500183
C	3.272173	-1.422531	-0.700441
H	2.963525	-2.095732	0.108642
H	2.931028	-1.833689	-1.658658
H	4.360711	-1.318410	-0.707787

I1b_full
E: -1202.937286
G: -1202.391030

Ti	0.079925	-0.011143	0.475890
N	0.232000	1.170143	-0.754271
N	1.887923	-0.588042	1.099339
N	-1.798918	-0.243670	1.243585
N	0.266611	1.007836	2.518517
Si	3.368868	-0.575613	0.125404
Si	-3.361049	-0.344648	0.434609
C	2.183495	-0.522910	2.526776
C	0.946456	-0.055490	3.283102
C	-1.090987	1.244008	3.037499
C	-1.979559	0.066678	2.662626
C	1.056882	2.243586	2.508029
H	3.019082	0.164614	2.750154
H	2.489379	-1.495630	2.946305
H	1.191728	0.287078	4.302347
H	0.244925	-0.890642	3.376203
H	-1.072294	1.430442	4.125674
H	-1.474282	2.141134	2.540936
H	-3.012823	0.351237	2.922388
H	-1.762962	-0.796981	3.315240
H	0.530672	2.997915	1.920872
H	1.215992	2.624070	3.530162
H	2.021397	2.061121	2.033713
C	-0.289578	-3.006357	-0.303117
C	-0.126525	-1.695743	-2.192916
C	-0.428765	-4.163774	-1.058210
H	-0.298046	-3.034835	0.782068
C	-0.256172	-2.804103	-3.024514

H	-0.004804	-0.691682	-2.584054
C	-0.410995	-4.060760	-2.448341
H	-0.547641	-5.121855	-0.563098
H	-0.236391	-2.673921	-4.101411
H	-0.516766	-4.945844	-3.069331
N	-0.142487	-1.792261	-0.855552
O	0.778569	1.955345	-1.723801
C	-0.070539	3.038468	-2.201916
C	-4.270464	1.329985	0.486894
H	-5.272105	1.247524	0.049463
H	-4.390557	1.705119	1.509050
H	-3.713862	2.082659	-0.081019
C	-3.257537	-0.869810	-1.381198
H	-2.564270	-0.247195	-1.951486
H	-2.953397	-1.915154	-1.485335
H	-4.251567	-0.765894	-1.831342
C	-4.472270	-1.626988	1.305900
H	-4.634436	-1.390332	2.362634
H	-5.456450	-1.677293	0.826119
H	-4.022401	-2.624535	1.253692
C	4.264586	1.095159	0.291754
H	4.495650	1.354542	1.330594
H	5.212786	1.082382	-0.257945
H	3.637703	1.886442	-0.131893
C	3.058063	-0.853785	-1.716294
H	2.635881	-1.841765	-1.918987
H	2.391510	-0.085038	-2.116732
H	4.014626	-0.784249	-2.247403
C	4.547846	-1.942702	0.735793
H	5.468049	-1.950954	0.140732
H	4.835686	-1.800672	1.782814
H	4.082609	-2.930616	0.647396
C	-0.415788	3.969713	-1.042570
H	-0.962750	3.417288	-0.273684
H	0.496336	4.380531	-0.598105
H	-1.038398	4.801905	-1.386815
C	0.812833	3.736100	-3.230722
H	0.287894	4.589803	-3.670336
H	1.733518	4.096912	-2.762797
H	1.084461	3.044882	-4.034366
C	-1.330701	2.469552	-2.846024
H	-1.072336	1.813161	-3.683849
H	-1.895390	1.893762	-2.109440
H	-1.969921	3.273604	-3.225108

I2

E: -600.905378

G: -600.686139

Ti	-0.043729	0.281304	0.583430
N	-0.137440	1.969891	0.367925
N	1.800653	-0.392484	0.609316
N	-1.698380	-0.809912	0.734570
N	0.060218	-0.277004	2.700903
Si	3.128250	0.361063	-0.249881
Si	-2.760841	-0.966800	-0.633130
C	2.140268	-1.235016	1.748917
C	0.880750	-1.512251	2.573763
C	-1.327249	-0.579248	3.125146
C	-2.066812	-1.355251	2.031262
C	0.690713	0.701867	3.599057
H	2.900757	-0.755247	2.389667
H	2.567223	-2.206102	1.452679
H	1.123186	-1.917560	3.567877
H	0.269477	-2.250827	2.047102
H	-1.331991	-1.116849	4.086900
H	-1.820820	0.386972	3.270265
H	-3.144530	-1.266414	2.243856
H	-1.840187	-2.432261	2.105971
H	0.085370	1.609668	3.617576
H	0.783493	0.299032	4.618876
H	1.679524	0.964689	3.221195
H	2.579509	1.167825	-1.377441
H	4.067404	-0.671181	-0.812293
H	3.953565	1.237691	0.652132
H	-2.060705	-0.283457	-1.772249
H	-3.019689	-2.392619	-1.033824
H	-4.104687	-0.323311	-0.430556
O	-0.277916	3.282551	0.111718
C	-1.646276	3.675588	0.100994
H	-2.199092	3.136121	-0.677296
H	-2.111733	3.483701	1.075863
H	-1.651582	4.747628	-0.111073

I3

E: -756.849574

G: -756.550648

Ti	0.024912	-0.103921	0.005686
N	0.770653	-0.555295	1.483595
O	1.377165	-0.965854	2.604592
N	-1.623549	-1.171197	-0.367411
N	0.679033	1.640975	-0.753593
N	-1.662818	1.343602	0.548086
Si	-1.736354	-2.875840	0.009241
Si	2.360107	2.002991	-1.041817
C	2.359573	-0.029453	3.052017

C	-2.913848	-0.504168	-0.470285
C	-2.690989	1.003192	-0.456731
C	-1.170971	2.722409	0.362997
C	-0.241814	2.767434	-0.844595
C	-2.165287	1.133848	1.912778
H	-3.591869	-0.782524	0.356933
H	-3.456497	-0.762857	-1.394636
H	-3.625898	1.554869	-0.265358
H	-2.311702	1.320224	-1.433558
H	-2.008904	3.434516	0.278928
H	-0.590499	2.978682	1.254540
H	0.270991	3.742890	-0.837770
H	-0.827568	2.754766	-1.779671
H	-1.373730	1.375870	2.623982
H	-3.044673	1.765221	2.115994
H	-2.429931	0.084860	2.050965
C	1.814047	-1.631718	-0.765634
C	1.143395	-1.232691	-1.717251
C	2.793086	-2.273299	0.108784
H	3.595296	-1.570976	0.357649
H	2.338270	-2.612129	1.042268
H	3.236866	-3.130756	-0.409662
C	0.559483	-0.977116	-3.038965
H	0.573231	0.093519	-3.262925
H	1.128208	-1.505580	-3.812670
H	-0.479452	-1.318812	-3.064142
H	3.258661	1.032748	-0.344409
H	2.750224	1.985283	-2.498465
H	2.683684	3.388066	-0.546044
H	-2.417528	-3.645268	-1.093834
H	-2.567905	-3.108339	1.243426
H	-0.384101	-3.468125	0.215865
H	2.802624	-0.462441	3.952141
H	1.889040	0.931600	3.287596
H	3.125525	0.122840	2.283979

TS3-4

E: -756.846673

G: -756.546091

Ti	0.018589	0.173413	0.107978
N	-0.147416	-0.824689	-1.327750
O	-0.080243	-1.548366	-2.435613
N	-1.682626	0.370648	1.148005
N	1.896093	0.475513	0.737477
N	0.250219	-1.320631	1.859474
Si	-3.249830	0.708136	0.450092
Si	3.131236	1.406617	-0.078409
C	1.274417	-1.804269	-2.839276

C	-1.771750	-0.119159	2.518170
C	-0.395285	-0.592347	2.966884
C	1.687313	-1.522285	2.097995
C	2.414860	-0.197343	1.927022
C	-0.428289	-2.595536	1.593542
H	-2.495780	-0.948778	2.617172
H	-2.114412	0.656000	3.223348
H	-0.452380	-1.217345	3.873410
H	0.227459	0.278037	3.195884
H	1.872100	-1.975391	3.086343
H	2.044646	-2.219012	1.332711
H	3.493496	-0.418391	1.856001
H	2.305265	0.424313	2.831409
H	0.055024	-3.089397	0.748093
H	-0.390088	-3.260580	2.470587
H	-1.468932	-2.411978	1.323430
C	-0.321573	1.307351	-1.843050
C	-0.169969	2.057177	-0.835135
C	-0.632270	1.114608	-3.269112
H	0.222918	0.722299	-3.827037
H	-1.464311	0.419537	-3.406916
H	-0.902544	2.084676	-3.700014
C	-0.178100	3.430455	-0.281974
H	0.802084	3.679612	0.137969
H	-0.428552	4.178820	-1.043036
H	-0.903577	3.500874	0.534801
H	2.640354	1.970121	-1.368806
H	3.638200	2.550852	0.761800
H	4.340018	0.552326	-0.360352
H	-3.988937	1.759196	1.237839
H	-4.136778	-0.509952	0.470702
H	-3.126795	1.181709	-0.957860
H	1.209364	-2.382122	-3.763783
H	1.792735	-2.378703	-2.065295
H	1.804984	-0.861849	-3.009203

I4

E: -756.876844

G: -756.575954

Ti	0.015721	0.071058	-0.079192
N	0.122301	-0.007304	1.867656
N	1.645437	-0.010453	-1.125929
N	-1.594718	-0.539453	-0.964832
N	0.415104	-2.313544	-0.271645
Si	2.367504	1.466969	-1.736709
Si	-2.937396	0.505527	-1.409711
C	2.387883	-1.256476	-1.265765
C	1.387419	-2.399526	-1.377806

C	-0.899623	-2.864815	-0.634701
C	-1.658565	-1.888908	-1.529381
C	0.949614	-2.943841	0.940673
H	3.068423	-1.428360	-0.415803
H	3.020776	-1.256358	-2.166309
H	1.882569	-3.384136	-1.388875
H	0.845977	-2.282489	-2.320958
H	-0.807908	-3.854986	-1.112217
H	-1.463166	-2.997930	0.294799
H	-2.696717	-2.249985	-1.609782
H	-1.253457	-1.910862	-2.553513
H	0.292075	-2.740846	1.787440
H	1.064981	-4.031566	0.811193
H	1.924699	-2.513507	1.178382
C	-0.106034	1.377166	1.830052
C	-0.074039	1.945404	0.561687
C	-0.317941	2.091753	3.141280
H	-1.321970	1.913167	3.540258
H	0.395052	1.720857	3.882468
H	-0.187829	3.167572	3.019435
C	-0.173544	3.414262	0.296679
H	-0.674984	3.602079	-0.658451
H	-0.727142	3.965524	1.068375
H	0.821401	3.872384	0.218282
H	-2.788977	1.840516	-0.766205
H	-3.037851	0.690506	-2.898353
H	-4.233965	-0.117818	-0.972837
H	3.231113	1.116233	-2.919336
H	3.252785	2.179150	-0.754141
H	1.313124	2.421881	-2.189302
O	-0.380406	-0.665249	2.997923
C	-1.778767	-0.903393	2.895492
H	-2.349546	0.031273	2.822700
H	-2.013625	-1.522745	2.021089
H	-2.058672	-1.429349	3.812012

TS4-5

E: -756.865151

G: -756.575954

Ti	0.187765	0.002905	0.048897
N	0.533992	1.690985	-0.899649
N	1.530422	-0.495494	1.343281
N	-1.516245	-0.941660	-0.198116
N	-0.893313	0.439827	2.078869
Si	3.190110	-0.741798	0.801264
Si	-1.975747	-1.854168	-1.625677
C	1.281157	-0.442758	2.778670
C	-0.222113	-0.483220	3.014184

C	-2.307462	0.085175	1.860975
C	-2.398486	-1.136981	0.954507
C	-0.747651	1.839424	2.504855
H	1.711247	0.465910	3.231660
H	1.739688	-1.288228	3.312659
H	-0.482013	-0.244662	4.057903
H	-0.580575	-1.494094	2.798787
H	-2.833557	-0.071429	2.816943
H	-2.776054	0.932811	1.351301
H	-3.450709	-1.251248	0.648761
H	-2.151339	-2.053504	1.514944
H	-1.135660	2.496026	1.723302
H	-1.282184	2.028069	3.448304
H	0.308947	2.075831	2.647727
C	0.824572	0.900532	-2.028222
C	1.267182	-0.342371	-1.633286
C	0.783479	1.454264	-3.433186
H	-0.083772	1.096817	-3.999503
H	0.769058	2.546711	-3.420266
H	1.678852	1.131128	-3.973237
C	1.926483	-1.322613	-2.552543
H	1.877217	-2.342077	-2.159308
H	1.480370	-1.329317	-3.556394
H	2.992092	-1.084650	-2.675274
H	-1.298501	-1.320709	-2.842769
H	-1.664336	-3.321027	-1.520104
H	-3.465594	-1.753992	-1.816240
H	4.023928	-0.978592	2.035335
H	3.787179	0.434696	0.095789
H	3.339420	-1.951933	-0.061757
O	-0.774152	2.354823	-0.816172
C	-1.696996	2.193713	-1.881507
H	-1.430982	2.798716	-2.755905
H	-1.807893	1.142646	-2.174791
H	-2.653660	2.548252	-1.487435

I5

E: -756.870648

G: -756.575954

Ti	0.096028	0.168851	0.128162
N	-0.891733	0.994153	1.601281
N	1.509534	1.385933	-0.373407
N	-0.377460	-1.471754	-0.888043
N	2.046805	-1.130441	0.344502
Si	1.099133	3.079638	-0.650800
Si	-1.924850	-1.933575	-1.566419
C	2.917886	1.020670	-0.422028
C	3.007697	-0.488466	-0.573987

C	1.690156	-2.486384	-0.108238
C	0.703841	-2.386618	-1.263814
C	2.563172	-1.135072	1.720005
H	3.455940	1.351251	0.481918
H	3.445606	1.485770	-1.268198
H	4.028127	-0.866072	-0.399930
H	2.718374	-0.751062	-1.595366
H	2.587832	-3.067261	-0.376884
H	1.196926	-2.992805	0.727535
H	0.334117	-3.402853	-1.477271
H	1.218106	-2.061772	-2.182746
H	1.807920	-1.544852	2.392532
H	3.485595	-1.730166	1.798141
H	2.775909	-0.112611	2.040010
C	-2.012346	1.033076	0.707684
C	-1.526541	1.283251	-0.537975
C	-3.430779	0.970553	1.215608
H	-3.920900	0.016841	0.986784
H	-3.454684	1.122992	2.298243
H	-4.030285	1.758332	0.747968
C	-2.301600	1.741420	-1.726520
H	-2.067735	1.133456	-2.607757
H	-3.389530	1.725555	-1.578455
H	-2.015532	2.768305	-1.986413
H	-3.060237	-1.251249	-0.880604
H	-2.038382	-1.648316	-3.038657
H	-2.110606	-3.420340	-1.417485
H	2.386193	3.863883	-0.619210
H	0.195272	3.652822	0.387860
H	0.495049	3.313826	-2.002041
O	-0.525114	-0.433503	2.091452
C	-1.579201	-1.339305	2.389611
H	-2.158739	-0.964455	3.239545
H	-2.235327	-1.511290	1.530951
H	-1.103352	-2.285504	2.663237

TS5-6

E: -756.869779

G: -756.575954

Ti	0.244479	0.007176	0.051092
N	0.484363	-1.030769	1.688456
N	1.690715	-0.605084	-1.094793
N	-0.904163	1.602866	-0.271518
N	-0.820647	-0.525039	-1.972018
Si	3.275258	-1.075335	-0.482386
Si	-1.199551	2.980859	0.773243
C	1.529082	-0.884706	-2.516356
C	0.220405	-0.270502	-2.984171

C	-1.951101	0.406287	-2.112829
C	-1.542632	1.771419	-1.580715
C	-1.264020	-1.925016	-2.014974
H	1.539439	-1.969414	-2.718258
H	2.347071	-0.459633	-3.120469
H	-0.086891	-0.651617	-3.971403
H	0.350077	0.812324	-3.065450
H	-2.304143	0.455730	-3.156158
H	-2.769774	0.021433	-1.496500
H	-2.451311	2.392663	-1.521883
H	-0.883397	2.286367	-2.298242
H	-1.989194	-2.099622	-1.218983
H	-1.716554	-2.169436	-2.988009
H	-0.414555	-2.588582	-1.841317
C	0.619898	0.168918	2.400449
C	1.313246	0.987924	1.555616
C	0.238329	0.301152	3.851504
H	-0.197195	1.281097	4.072341
H	-0.470575	-0.478121	4.141339
H	1.128333	0.184346	4.481727
C	2.161316	2.155961	1.913580
H	2.007042	2.987779	1.217607
H	2.007824	2.519784	2.938360
H	3.219173	1.875197	1.817621
H	-0.897929	2.686284	2.203149
H	-0.408671	4.198448	0.379093
H	-2.647686	3.379118	0.672457
H	3.539086	-2.522816	-0.796487
H	3.407877	-0.862954	0.982054
H	4.348911	-0.294397	-1.191629
O	-1.093643	-1.256181	1.039382
C	-2.177153	-0.779012	1.806810
H	-2.395637	-1.479924	2.621489
H	-1.988598	0.218722	2.222863
H	-3.054690	-0.706467	1.152669

I6

E: -756.924567

G: -756.621337

Ti	-0.106963	-0.165898	0.135034
N	-1.398065	1.466292	0.732427
N	1.224777	1.250349	-0.157771
N	-0.367871	-1.683571	-1.126252
N	1.912901	-1.259219	0.162395
Si	0.997250	2.928378	0.348938
Si	-1.907831	-1.971087	-1.896898
C	2.575426	0.940841	-0.622067
C	2.663246	-0.555335	-0.889984

C	1.633664	-2.663261	-0.175699
C	0.654746	-2.702685	-1.335589
C	2.591659	-1.160578	1.459491
H	3.340038	1.234560	0.115670
H	2.836189	1.477024	-1.546991
H	3.707482	-0.904258	-0.939556
H	2.182235	-0.779216	-1.845898
H	2.562351	-3.216078	-0.394159
H	1.164141	-3.109336	0.706278
H	0.229550	-3.715815	-1.391358
H	1.189687	-2.558663	-2.290639
H	1.988148	-1.670560	2.211192
H	3.591882	-1.618068	1.417637
H	2.687953	-0.113350	1.750650
C	-2.537359	0.972699	0.397608
C	-1.762174	0.786155	-0.766912
C	-3.883969	0.881306	0.991912
H	-4.162783	-0.175578	1.062020
H	-3.909464	1.335865	1.984428
H	-4.616542	1.364598	0.337570
C	-1.936483	1.647554	-1.988613
H	-1.059047	1.597956	-2.637197
H	-2.802269	1.304015	-2.566130
H	-2.106844	2.695306	-1.711514
H	-3.082513	-1.834864	-0.973267
H	-2.187695	-1.098848	-3.086745
H	-1.933606	-3.390586	-2.405163
H	0.742446	3.092994	1.814285
H	-0.067482	3.656317	-0.406738
H	2.292639	3.639190	0.055146
O	-0.424363	-0.890374	1.794946
C	-0.665598	-0.440924	3.093407
H	0.270324	-0.343193	3.664148
H	-1.157133	0.543705	3.095058
H	-1.308395	-1.154909	3.627685

TS6-7

E: -756.900237

G: -756.594095

Ti	0.002542	0.143210	0.032670
N	-1.502841	1.463294	0.425974
N	1.073665	1.689314	-0.482786
N	0.227304	-1.483005	-1.066511
N	2.167437	-0.535020	0.594333
Si	0.321100	3.228247	-0.917428
Si	-1.046616	-2.166850	-2.051618
C	2.513403	1.731147	-0.274772
C	3.041190	0.308497	-0.252534

C	2.259008	-1.951321	0.196733
C	1.525757	-2.150900	-1.122765
C	2.485467	-0.346204	2.015238
H	2.775529	2.247750	0.665532
H	3.036038	2.282115	-1.071581
H	4.085096	0.252279	0.095043
H	3.002518	-0.087831	-1.269964
H	3.309787	-2.280107	0.138381
H	1.764045	-2.543476	0.973111
H	1.423884	-3.233306	-1.292020
H	2.142221	-1.784227	-1.960227
H	1.770193	-0.895711	2.629900
H	3.504475	-0.691797	2.244932
H	2.407303	0.712109	2.274861
C	-2.104198	0.444053	1.080350
C	-2.048993	0.243988	-0.334870
C	-3.092272	0.480297	2.188152
H	-3.444307	-0.517633	2.458853
H	-2.668227	0.975047	3.065285
H	-3.951268	1.062790	1.839446
C	-3.218070	0.371448	-1.270809
H	-2.897401	0.758947	-2.241747
H	-3.691740	-0.600028	-1.443419
H	-3.976483	1.056017	-0.869076
H	-2.226846	-2.633911	-1.251463
H	-1.552007	-1.239013	-3.110659
H	-0.506584	-3.384482	-2.758599
H	-0.017868	4.099148	0.253435
H	-0.879553	3.049032	-1.780793
H	1.345493	3.983752	-1.726193
O	-0.696573	-0.486335	1.801177
C	-0.990893	-1.831628	2.125444
H	-1.584346	-1.871668	3.047347
H	-1.537553	-2.329472	1.315556
H	-0.060176	-2.383470	2.302133

TS6-11

E: -756.900479

G: -756.598355

Ti	-0.154714	-0.083772	0.255567
N	-1.266203	1.496820	0.670148
N	1.205501	1.287608	-0.200867
N	-0.576134	-1.542399	-1.076639
N	1.811394	-1.250576	0.220973
Si	1.056276	2.976302	0.287167
Si	-1.906015	-1.809013	-2.177830
C	2.536063	0.896561	-0.657339
C	2.550980	-0.609834	-0.878994

C	1.393319	-2.627612	-0.080929
C	0.402795	-2.626942	-1.234687
C	2.564719	-1.195828	1.476988
H	3.320994	1.177248	0.064412
H	2.818655	1.386353	-1.602175
H	3.575945	-1.006918	-0.957614
H	2.024048	-0.835888	-1.809381
H	2.260363	-3.275105	-0.293965
H	0.895779	-3.003947	0.818635
H	-0.080161	-3.618379	-1.249282
H	0.942506	-2.554206	-2.195623
H	1.960092	-1.638002	2.270007
H	3.517616	-1.740497	1.392396
H	2.769733	-0.156907	1.741671
C	-2.442658	0.652923	0.322203
C	-1.896580	1.284939	-0.679425
C	-3.584829	0.051711	1.024298
H	-3.253852	-0.725238	1.717048
H	-4.078480	0.838709	1.609877
H	-4.303097	-0.369520	0.317172
C	-1.954816	1.987892	-1.969720
H	-0.966438	2.050256	-2.430677
H	-2.651444	1.495842	-2.652406
H	-2.300639	3.013335	-1.786067
H	-3.059383	-0.891295	-1.939561
H	-1.504470	-1.648232	-3.622316
H	-2.416844	-3.220268	-2.056352
H	0.818324	3.189193	1.748570
H	0.030004	3.747158	-0.482650
H	2.380423	3.626463	-0.028138
O	-0.398753	-0.743577	1.948175
C	-0.563265	-0.197236	3.225185
H	0.401959	-0.098340	3.743413
H	-1.022700	0.800222	3.175200
H	-1.201728	-0.851155	3.836318

I7
E: -756.906082
G: -756.59899

Ti	0.069567	0.228829	0.010563
N	-1.417911	1.349702	0.672549
N	1.140622	1.697180	-0.663867
N	0.230332	-1.452325	-1.023013
N	2.188003	-0.473174	0.638668
Si	0.410274	3.169314	-1.294718
Si	-1.059157	-2.108773	-1.999822
C	2.548127	1.779364	-0.299567

C	3.100029	0.368696	-0.178282
C	2.276438	-1.889528	0.222922
C	1.543766	-2.081274	-1.101905
C	2.472074	-0.305413	2.070772
H	2.693489	2.329743	0.646706
H	3.145520	2.316339	-1.053584
H	4.116610	0.350073	0.244226
H	3.142550	-0.065006	-1.179926
H	3.328464	-2.213358	0.165601
H	1.781878	-2.489317	0.993893
H	1.476034	-3.163118	-1.293863
H	2.151799	-1.678077	-1.929688
H	1.726950	-0.842738	2.661842
H	3.474150	-0.679659	2.327375
H	2.418179	0.753294	2.338013
C	-1.999165	0.201910	1.276003
C	-2.002295	0.292950	-0.184985
C	-3.123993	0.314483	2.262640
H	-3.643015	-0.637216	2.416674
H	-2.750274	0.676189	3.226181
H	-3.848544	1.037998	1.882971
C	-3.189091	0.536226	-1.072029
H	-2.893762	1.090785	-1.968214
H	-3.637636	-0.406675	-1.401140
H	-3.963733	1.122867	-0.560573
H	-2.249290	-2.550213	-1.199200
H	-1.555451	-1.172430	-3.057575
H	-0.549066	-3.339585	-2.709849
H	0.282417	4.251990	-0.263951
H	-0.928128	2.864700	-1.871618
H	1.294776	3.710200	-2.384975
O	-0.867438	-0.627825	1.797341
C	-1.165248	-2.012648	1.971823
H	-1.868052	-2.138145	2.802068
H	-1.579334	-2.439401	1.054036
H	-0.232825	-2.521847	2.223527

I8

E: -756.906702

G: -756.602222

Ti	-0.280740	0.191270	0.197333
N	-0.854204	-1.190841	-1.063302
O	1.103602	-0.245062	-2.181348
N	-1.623266	0.603817	1.519487
N	1.528006	0.697292	0.719567
N	0.141319	-1.477519	1.771815
Si	-2.312920	2.204368	1.573629
Si	2.477123	1.930590	-0.078902

C	2.077689	-1.273323	-2.184092
C	-1.958889	-0.422115	2.498805
C	-0.654107	-1.065655	2.955885
C	1.596628	-1.359777	2.022965
C	2.044432	0.098749	1.946905
C	-0.214530	-2.844702	1.368793
H	-2.633275	-1.179286	2.070184
H	-2.474270	-0.010844	3.379733
H	-0.819469	-1.924624	3.624184
H	-0.082456	-0.313344	3.506587
H	1.866558	-1.820527	2.987561
H	2.103450	-1.917449	1.228938
H	3.145529	0.102733	1.983076
H	1.714655	0.650370	2.842413
H	0.290416	-3.093602	0.434845
H	0.061714	-3.569543	2.149566
H	-1.287123	-2.904076	1.178141
C	-0.241790	-0.706423	-2.295626
C	-1.206041	0.147485	-1.608589
C	-0.514142	-1.462590	-3.573962
H	-0.199202	-0.873440	-4.441459
H	0.016712	-2.419770	-3.592981
H	-1.580066	-1.680112	-3.662383
C	-2.592448	0.508505	-2.067054
H	-3.281917	0.545233	-1.217246
H	-2.597323	1.494780	-2.543829
H	-2.995257	-0.215643	-2.787271
H	1.636012	2.587830	-1.121266
H	2.924798	2.978147	0.902848
H	3.728097	1.387460	-0.711816
H	-2.154005	2.837954	2.925898
H	-3.773777	2.256286	1.231407
H	-1.557937	3.003173	0.554762
H	3.018812	-0.819179	-1.868251
H	2.213085	-1.705524	-3.183853
H	1.816045	-2.078690	-1.483049

I9

E: -756.910390

G: -756.602222

Ti	-0.224159	-0.410328	-0.177665
N	-1.331512	-0.951103	1.283268
O	0.332279	0.576430	2.168968
N	-0.957586	-0.835545	-1.894244
N	1.723778	-0.713158	-0.367896
N	0.397841	1.508450	-1.225995
Si	-2.348946	-1.786090	-2.369998
Si	2.396306	-2.292035	-0.070443

C	-0.091333	-0.273097	-2.937104
C	0.124763	1.221082	-2.665423
C	1.843434	1.639488	-0.917507
C	2.554505	0.295986	-1.005337
C	-0.284500	2.749271	-0.818974
H	-0.539136	-0.360533	-3.939138
H	0.865503	-0.808904	-2.976381
H	-0.804225	1.739018	-2.919571
H	0.921792	1.637516	-3.298997
H	2.310180	2.392672	-1.572651
H	1.904600	1.999381	0.114040
H	3.539659	0.412022	-0.523526
H	2.765915	0.048879	-2.060234
H	-0.130530	2.910212	0.249324
H	0.100838	3.615571	-1.379578
H	-1.355195	2.649843	-0.998250
C	-1.038466	0.142946	2.207767
C	-1.723272	0.448415	0.962513
C	-1.642123	0.114656	3.587628
H	-1.512702	1.083034	4.082424
H	-2.709400	-0.104574	3.517839
H	-1.188286	-0.660209	4.213325
C	-3.147406	0.893087	0.797188
H	-3.799647	0.527370	1.601828
H	-3.211145	1.987594	0.792015
H	-3.560565	0.533173	-0.150477
H	3.537969	-2.277133	0.909504
H	1.292107	-3.132466	0.493359
H	2.919546	-2.954226	-1.316076
H	-3.249328	-0.992865	-3.276127
H	-3.095689	-2.189960	-1.146173
H	-1.953218	-3.015208	-3.138095
C	1.219245	-0.189049	2.975012
H	1.066301	-1.266446	2.831435
H	2.233161	0.068207	2.664349
H	1.099377	0.052593	4.038155

TS9-10

E: -756.874550

G: -756.572344

Ti	-0.217104	-0.492475	-0.437391
N	-1.104546	-1.177336	0.947362
O	0.393092	0.357724	2.569866
N	-1.124314	-0.734614	-2.148831
N	1.722975	-0.828081	-0.544896
N	0.404733	1.512996	-1.387026
Si	-2.422757	-1.796514	-2.630638
Si	2.612342	-2.140392	0.178267

C	-0.353916	-0.068792	-3.200794
C	-0.077665	1.382068	-2.791865
C	1.884961	1.491768	-1.276640
C	2.461852	0.085369	-1.411624
C	-0.102659	2.764406	-0.801741
H	-0.903044	-0.026888	-4.155650
H	0.583759	-0.599398	-3.422645
H	-1.029081	1.918739	-2.848255
H	0.624976	1.872525	-3.483760
H	2.332938	2.187877	-2.005397
H	2.125634	1.850158	-0.270763
H	3.527768	0.154471	-1.136836
H	2.451909	-0.235793	-2.465480
H	0.216979	2.832568	0.239592
H	0.266238	3.645411	-1.351371
H	-1.193717	2.761658	-0.822639
C	-0.932793	0.296536	2.442174
C	-1.465471	0.230640	1.130184
C	-1.754298	0.282348	3.692732
H	-1.435534	1.066448	4.388747
H	-2.809203	0.420168	3.458292
H	-1.646412	-0.680765	4.204781
C	-2.887299	0.684920	0.869379
H	-3.629931	0.073145	1.402718
H	-3.031356	1.734627	1.155072
H	-3.116054	0.596266	-0.196365
H	3.746483	-1.636438	1.036044
H	1.688181	-2.952098	1.022800
H	3.254803	-3.047773	-0.837332
H	-3.355825	-1.084610	-3.576016
H	-3.178321	-2.240028	-1.425415
H	-1.947543	-3.016693	-3.374205
C	1.030926	-0.240953	3.699218
H	0.835970	-1.317670	3.709374
H	2.097160	-0.065217	3.560674
H	0.705893	0.213657	4.640376

I10

E: -756.943695

G: -756.638605

Ti	0.029416	0.006717	-0.321123
N	0.908370	-0.890915	-1.573943
O	2.014411	0.010781	0.640003
N	-1.760063	-0.768896	-0.277316
N	-0.214652	1.904048	-0.637750
N	-0.620740	0.579582	1.872448
Si	-2.447447	-1.814224	-1.500696
Si	-0.027875	2.740088	-2.166303

C	-2.679781	-0.021628	0.573351
C	-2.046177	0.168511	1.951642
C	-0.430034	2.049833	1.812437
C	-0.799993	2.666824	0.463502
C	0.106271	0.054660	3.037489
H	-3.629903	-0.558185	0.724236
H	-2.951177	0.949220	0.133103
H	-2.062149	-0.803099	2.453799
H	-2.617912	0.876476	2.572419
H	-0.984981	2.541606	2.629052
H	0.637179	2.225996	1.981897
H	-0.424246	3.703444	0.485919
H	-1.893131	2.752663	0.368730
H	1.163636	0.308821	2.950212
H	-0.289069	0.465546	3.979410
H	0.011922	-1.033340	3.062409
C	2.055065	-1.399421	0.424266
C	1.535577	-1.811263	-0.792593
C	2.772120	-2.156935	1.489908
H	2.319698	-2.001418	2.476566
H	2.761947	-3.229243	1.288134
H	3.823957	-1.846274	1.568196
C	1.569690	-3.252016	-1.240389
H	2.023203	-3.290732	-2.235586
H	2.135286	-3.906434	-0.573716
H	0.551039	-3.637561	-1.335700
H	0.884123	3.927610	-2.008708
H	0.542265	1.801028	-3.170936
H	-1.333334	3.287171	-2.675268
H	-3.749946	-2.363063	-0.978141
H	-1.545745	-2.961570	-1.809137
H	-2.766341	-1.121514	-2.795670
C	3.106261	0.720938	0.024811
H	3.099809	0.547061	-1.054834
H	2.952107	1.780586	0.233444
H	4.049782	0.386452	0.466693

I11

E: -756.924562

G: -756.621844

Ti	-0.003274	0.017186	0.273329
N	1.161715	-1.780814	0.297928
N	-1.177005	-1.043281	-0.930255
N	0.460920	1.814729	-0.437052
N	-2.001006	1.212963	0.282231
Si	-1.067885	-2.782256	-1.167114
Si	1.968518	2.105189	-1.268903
C	-2.432515	-0.470407	-1.422617

C	-2.478492	1.014154	-1.095931
C	-1.607883	2.597782	0.563529
C	-0.424481	2.968650	-0.318396
C	-2.979418	0.737132	1.262619
H	-3.312020	-0.973587	-0.987403
H	-2.539894	-0.583750	-2.512354
H	-3.489686	1.431135	-1.234189
H	-1.794139	1.541014	-1.764035
H	-2.450241	3.296753	0.429214
H	-1.304055	2.625854	1.615318
H	0.075141	3.838126	0.137115
H	-0.778242	3.317712	-1.303388
H	-2.566687	0.864950	2.264037
H	-3.926923	1.291829	1.180126
H	-3.175222	-0.325693	1.109247
C	2.068567	-0.373987	0.389826
C	2.143823	-1.470853	-0.483452
C	3.045092	-0.135635	1.506467
H	2.671817	0.621430	2.199164
H	3.224976	-1.063673	2.065344
H	4.005900	0.210018	1.107477
C	2.921622	-2.121790	-1.553162
H	2.774178	-1.557213	-2.480493
H	3.989479	-2.080532	-1.317124
H	2.601573	-3.153915	-1.703000
H	2.309717	1.031251	-2.258761
H	1.849846	3.384250	-2.058484
H	3.160650	2.277127	-0.371282
H	-1.170610	-3.596701	0.086288
H	0.170470	-3.212134	-1.891860
H	-2.223429	-3.192932	-2.040868
O	-0.261975	-0.051619	2.070625
C	-0.321969	-1.022851	3.076376
H	-1.362278	-1.319991	3.273611
H	0.242475	-1.922761	2.797926
H	0.096441	-0.621684	4.009425

TS11-12

E: -756.889729

G: -756.588754

Ti	0.029545	0.063838	0.533548
N	-1.747240	1.085844	1.049727
N	0.421621	1.750779	-0.420486
N	-0.244692	-1.528527	-0.813974
N	2.212143	-0.457453	-0.262674
Si	-0.564522	3.204031	-0.504240
Si	-0.926258	-1.626146	-2.417305
C	1.821132	1.911214	-0.821382

C	2.379013	0.578912	-1.304350
C	2.170022	-1.837955	-0.810448
C	0.815006	-2.479898	-0.487030
C	3.250120	-0.333799	0.769627
H	2.449534	2.308033	-0.005675
H	1.922239	2.632211	-1.647306
H	3.436533	0.667892	-1.605187
H	1.798028	0.268127	-2.177206
H	2.305124	-1.801207	-1.896668
H	2.994936	-2.434537	-0.401578
H	0.778670	-2.727538	0.585648
H	0.719371	-3.438524	-1.022134
H	3.051245	-1.045135	1.571744
H	4.250320	-0.514670	0.346565
H	3.225196	0.665679	1.206738
C	-1.668821	-0.948034	0.635284
C	-2.401835	0.257615	0.301784
C	-2.263270	-2.138341	1.295432
H	-1.519895	-2.919456	1.471362
H	-2.651140	-1.819940	2.271675
H	-3.106393	-2.561598	0.733349
C	-3.654291	0.500828	-0.486125
H	-3.409464	0.918449	-1.468063
H	-4.223900	-0.420243	-0.638629
H	-4.270063	1.235741	0.039575
H	-1.631837	-2.936175	-2.635622
H	-1.892507	-0.511702	-2.622125
H	0.125495	-1.540035	-3.491764
H	-0.644528	3.998081	0.765222
H	-1.954618	2.934075	-0.980945
H	0.076896	4.109149	-1.526442
O	0.732714	-0.239642	2.180167
C	0.470348	0.091473	3.515918
H	1.342387	0.586513	3.965349
H	-0.389999	0.767451	3.597993
H	0.260286	-0.815268	4.100189

I12

E: -756.971547

G: -756.666068

Ti	-0.101073	0.546131	0.438039
N	-1.879301	0.644930	0.549158
N	0.763037	2.053203	-0.439967
N	-0.631763	-0.871171	-1.252007
N	1.934136	-0.529313	-0.123975
Si	0.084696	3.624895	-0.792851
Si	-1.724856	-0.199364	-2.537548
C	2.214403	1.908023	-0.526242

C	2.558566	0.496657	-0.998756
C	1.648111	-1.777042	-0.839960
C	0.498661	-1.611111	-1.828864
C	2.800166	-0.802855	1.032760
H	2.700553	2.112566	0.441777
H	2.660921	2.610737	-1.248375
H	3.647757	0.337193	-1.050623
H	2.154039	0.381909	-2.007530
H	2.535910	-2.154916	-1.374435
H	1.382295	-2.522590	-0.084215
H	0.203198	-2.606149	-2.190662
H	0.835292	-1.051740	-2.709014
H	2.293369	-1.485424	1.716396
H	3.756511	-1.242569	0.708954
H	2.986686	0.121425	1.578409
C	-1.383694	-1.548438	-0.187960
C	-2.109868	-0.688124	0.634877
C	-1.509368	-3.042253	-0.223704
H	-0.549966	-3.566917	-0.126097
H	-2.138783	-3.389223	0.597329
H	-1.966943	-3.391173	-1.161027
C	-3.074999	-1.199339	1.683726
H	-3.738188	-0.380110	1.967380
H	-3.684739	-2.034947	1.326411
H	-2.541689	-1.526507	2.583217
H	-2.187531	-1.358970	-3.369715
H	-2.879069	0.505398	-1.940277
H	-0.899574	0.695043	-3.401403
H	0.526861	4.687992	0.176651
H	-1.402453	3.536721	-0.765421
H	0.538129	4.094317	-2.149629
O	0.505846	0.502087	2.180007
C	-0.112714	0.790650	3.402129
H	0.367517	1.655823	3.882376
H	-1.179929	1.021223	3.271314
H	-0.024035	-0.062086	4.092168

TS12-13

E: -756.966739

G: -756.659075

Ti	-0.132475	-0.380182	0.419442
N	0.863492	-1.739748	-0.351127
N	-1.986704	-0.643479	-0.078687
N	0.945052	0.519825	-1.218429
N	-0.879204	1.895510	0.328887
Si	-2.753327	-2.196454	-0.392597
Si	0.624441	-0.997809	-2.375818
C	-2.892376	0.497797	0.022588

C	-2.155393	1.760840	-0.408685
C	0.106838	2.690174	-0.423097
C	0.682382	1.895345	-1.601047
C	-1.109950	2.479044	1.657308
H	-3.288137	0.611123	1.045018
H	-3.771234	0.388419	-0.632972
H	-2.773431	2.663525	-0.274652
H	-1.924819	1.664528	-1.473061
H	-0.327430	3.639376	-0.777300
H	0.907979	2.945833	0.278109
H	1.580561	2.408028	-1.971055
H	-0.017706	1.864192	-2.441286
H	-0.174563	2.490911	2.218988
H	-1.506153	3.503361	1.578586
H	-1.817711	1.862773	2.213093
C	2.092116	0.218519	-0.392827
C	2.040496	-1.098336	0.019828
C	3.228883	1.181634	-0.267232
H	2.929850	2.158741	0.130108
H	3.993765	0.781958	0.400818
H	3.703095	1.359364	-1.241551
C	3.106075	-1.852946	0.755100
H	2.669266	-2.397148	1.597149
H	3.543676	-2.600679	0.083438
H	3.910556	-1.213069	1.126447
H	1.929162	-1.591095	-2.803905
H	0.271312	-0.053791	-3.528819
H	-0.532294	-1.943245	-2.487348
H	-1.736721	-3.280764	-0.377617
H	-3.474293	-2.172808	-1.710084
H	-3.795236	-2.481604	0.654319
O	0.025628	-0.275793	2.235625
C	0.814740	-0.660777	3.319247
H	0.744019	-1.742786	3.499522
H	1.874051	-0.410015	3.160532
H	0.478081	-0.147436	4.230778

I13

E: -757.019015

G: -756.714625

Ti	-0.113914	0.058896	0.449528
N	0.914332	-1.366181	-0.391993
N	-1.918307	-0.463559	-0.084269
N	1.190568	1.200665	-0.392226
N	-1.208973	2.069511	-0.018952
Si	-2.796717	-1.743826	0.736833
Si	0.312268	-2.590682	-1.491304
C	-2.713447	0.389574	-0.959603

C	-1.931700	1.675501	-1.241350
C	-0.196406	3.115006	-0.261016
C	1.017207	2.510416	-0.959874
C	-2.135077	2.479752	1.044682
H	-3.687297	0.641318	-0.504666
H	-2.946005	-0.096738	-1.918791
H	-2.595973	2.481173	-1.594308
H	-1.183054	1.489254	-2.018573
H	-0.620769	3.963821	-0.819797
H	0.114772	3.480680	0.722511
H	1.882097	3.169448	-0.797941
H	0.866343	2.466086	-2.052868
H	-1.566271	2.699148	1.950874
H	-2.709441	3.373291	0.754957
H	-2.825084	1.665793	1.269841
C	2.389085	0.485797	-0.413067
C	2.240636	-0.882562	-0.383829
C	3.688130	1.238321	-0.351199
H	3.724000	1.897976	0.526023
H	4.549041	0.570922	-0.300316
H	3.824335	1.871970	-1.236582
C	3.356670	-1.875131	-0.219790
H	3.249293	-2.423694	0.724505
H	3.337713	-2.622614	-1.020544
H	4.343132	-1.407936	-0.228445
H	1.375637	-3.594612	-1.828013
H	-0.162769	-2.025898	-2.800719
H	-0.824773	-3.325271	-0.863721
H	-1.865070	-2.485525	1.631752
H	-3.437007	-2.702271	-0.224853
H	-3.917481	-1.156604	1.553974
O	0.114396	-0.018527	2.239401
C	1.026369	-0.207711	3.280136
H	0.686107	-1.014996	3.942023
H	2.023072	-0.471872	2.900909
H	1.120398	0.708170	3.879907