C-H and H-H Activation at a Di-titanium Centre

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Supplementary Information

General Experimental: All manipulations were carried out in a MBraun glovebox under N_2 or Ar (O_2 and H_2O <1 ppm) or by using standard Schlenk techniques under Ar (BOC pureshield) passed through a column containing BASF R3-11(G) catalyst and activated molecular sieves (4 Å). All glassware was dried at 160 °C overnight prior to use. Filter cannulas were prepared using Whatman 25 mm glass microfiber filters and were pre-dried at 160 °C overnight. Toluene was dried over molten K, distilled under a N_2 atmosphere and kept in a Young's ampules over a potassium mirror under Ar. Hydrocarbons were dried over NaK, distilled under a N_2 atmosphere, and kept in Young's ampules over a potassium mirror under Ar. Deuterated toluene, and THF were degassed by three freeze−thaw cycles, dried by refluxing over molten K for 3 days, vacuum distilled, and kept in Young's ampoules in the glovebox under N_2. $Ti_2(\mu{:}\eta^5,\eta^5\text{-}Pn^\dagger)_2$ ($Pn^\dagger$ = $C_8H_4(1,4\text{-}Si^iPr_3)_2$) (**1**)[1] and 1,3,4,5-tetramethyl-imidazolium-2-ylidene (**2**)[2] were prepared according to published procedures and were stored in a glovebox freezer (-35 ºC) under N_2. ^{1}H-NMR, $^{13}C\{^1H\}$-NMR, DEPT135 $^{29}Si\{^1H\}$-NMR, deuterium spectra, correlation experiments, T_1 measurements (inversion method) and variable temperature experiments were recorded on a Varian VNMR S400 spectrometer operating at 400 MHz (^{1}H) at 30 °C unless otherwise stated. The spectra were referenced internally to the residual protic solvent (^{1}H) or the signals of the solvent (^{13}C). $^{29}Si\{^1H\}$ NMR spectra were referenced externally relative to $SiMe_4$. EI-MS mass spectra were recorded on a VG-Autospec Fisons instrument at the University of Sussex unless otherwise stated. IR spectra were recorded on a Perkin Elmer 100 instrument as thin films. Elemental analyses were performed at the Microanalysis Service of the School of Chemistry at University of Bristol.

Synthesis of (**3**): In a N_2 filled glovebox, a Young's ampoule was charged with 200 mg (0.216 mmol) of (**1**). A second Young's ampule was charged with 27 mg (1 mol. eq.) (**2**). The contents of these two ampoules were dissolved in toluene (*ca* 10 mL for (**1**) and 2-3 mL for (**2**)), and the solution of (**2**) was added dropwise to the solution of (**1**) cooled at 0 °C, with stirring over *ca* 10 minutes, and a colour change from crimson red to dark pine green was observed. After the addition was complete, the ice bath was removed and the reaction mixture stirred at RT for ca 90 minutes. The solvent was slowly removed under vacuum (ampoule tilted horizontally) with no stirring, to induce crystallisation of the title compound at an approximate volume of *ca* 0.5-1.5 mL. The crystals were taken in an Ar glovebox, separated from the mother liquor using a drown-out pipette and were washed with minimum amount of n-C_5 (3x1 mL) before being dried under vacuum. The mother-liquor and the n-C_5 washing were combined and chilled at -35 ºC to produce a second minute crop of (**3**). ^{1}H-NMR (δC_4D_8O): -7.91 (s, 1H, Ti*H*Ti), -2.91 (dd, J_{HH} = 12.91 Hz, J_{HH} = 12.32 , 1H, TiC*H*H), 0.90-1.27 (m, 68H, aliphatic), 1.28-1.41 (m, 5H, aliphatic), 1.41-1.81 (m, 12H, aliphatic), 1.80 (s, 3H, CH_3 ylidene), 1.98 (br m, 1H, C*H*$(CH_3)_2$), 2.13 (s, 3H CH_3 ylidene), 4.27 (s, 3H CH_3 ylidene), 5.34 (d, $^3J_{HH}$ = 2.93 Hz, 1H, Pn-*H*), 5.42 (d, $^3J_{HH}$ = 3.23 Hz, 1H, Pn-*H*), 5.62 (d, $^3J_{HH}$ = 2.93 Hz, 1H, Pn-*H*), 5.81 (d, $^3J_{HH}$ = 2.64 Hz, 1H, Pn-*H*), 6.71 (d, $^3J_{HH}$ = 2.93 Hz, 1H, Pn-*H*), 7.05 (d, $^3J_{HH}$ = 3.23 Hz, 1H, Pn-*H*), 7.09 (d, $^3J_{HH}$ = 2.35 Hz, 1H, Pn-*H*), 7.47 (d, $^3J_{HH}$ = 2.93 Hz, 1H, Pn-*H*); $^{13}C\{^1H\}$-NMR (δC_4D_8O): 8.69, 9.39, 12.33, 13.95, 15.09, 15.33, 16.82, 19.61, 20.31, 20.54, 20.66, 20.80, 21.00, 33,36, 35.14 (*C*H and *C*H_3's), 38.93 (N-*C*H_3), 49.23 (Ti*C*H_2), {92.36, 93.26, 100.04, 102.45 (aromatic quaternary)}, {103.05, 104.24, 107.49, 113.21 (aromatic CH)}, {102.29, 120.85 (aromatic quaternary)}, 126.40 (aromatic CH), 127.26 (aromatic quaternary), {127.33, 130.74 (aromatic CH)}, 131.40 (aromatic quaternary), 132.53 (aromatic CH), 134.52 (aromatic quaternary), 197.78 (N*C*N) (One aromatic quaternary could not be located);); ^{1}H-NMR (δC_7D_8): -7.81 (s, 1H, Ti*H*Ti), -2.57 (dd, J_{HH} = 12.91 Hz, J_{HH} = 12.32 , 1H, TiC*H*H), 1.02 (m, 4H, aliphatic), 1.06-1.38 (m, 68H, aliphatic), 1.45-1.56 (m, 8H, aliphatic), 1.56-1.68 (m, 6H, aliphatic), 1.69-178 (br d, 4H, aliphatic), 1.99 (br m, 1H, C*H*$(CH_3)_2$), 2.2 (m, 2H, aliphatic), 4.15 (s, 3H, CH_3 ylidene), 5.25 (d, $^3J_{HH}$ = 3.23 Hz, 1H, Pn-*H*), 5.57 (d, $^3J_{HH}$ = 3.23 Hz, 1H, Pn-*H*), 5.80 (d, $^3J_{HH}$ = 2.64 Hz, 1H, Pn-*H*), 5.93 (d, $^3J_{HH}$ = 2.64 Hz, 1H, Pn-*H*), 6.78 (d, $^3J_{HH}$ = 3.23 Hz, 1H, Pn-*H*), 7.20 (d, $^3J_{HH}$ = 3.23 Hz, 1H, Pn-*H*), 7.31 (d, $^3J_{HH}$ = 2.64 Hz, 1H, Pn-*H*), 7.63 (d, $^3J_{HH}$ = 2.93 Hz, 1H, Pn-*H*); $^{29}Si\{^1H\}$-NMR (δC_7D_8): 0.28, 2.26, 2.97, 4.94. EI. Anal.: Calcd for $C_{59}H_{104}N_2Si_4Ti_2$ **.** 0.5 C_7H_8: C 68.52, H 9.94, N, 2.56; Found C 68.36, H 10.14, N 2.74; Yield: 180 mg (*ca* 76%).

Synthesis of (**4**):
In a N_2 filled glovebox, a Young's NMR tube was charged with 18 mg (0.016 mmol) of (**3**).0.5C_7H_8 and dissolved in ca 0.5-0.7 mL C_7D_8 and the solution shaken well to dissolve most of (**3**). It was then freeze-thaw-degassed three times and exposed to 2 bar H_2 to produce (**4**) in a 100 % spectroscopic yield. ^{1}H-NMR (δC_7D_8): -8.82 (br s, 2H, Ti*H*Ti*H*), 0.96-1.15 (m, 30H, aliphatic), 1.17-1.24 (br d, 12H), 1.25-1.36 (m, 31H, aliphatic), 1.39 (br d., 8H, aliphatic), 1.53 (s, 3H, NHC-CH_3), 1.58 (m, 6H, aliphatic), 1.71 (m, 3H, aliphatic), 4.13 (s, 3H, NHC-CH_3), 5.27 (d, $^3J_{HH}$ = 3.23 Hz, 1H, Pn-*H*),5.35 (d, $^3J_{HH}$ = 2.93 Hz, 1H, Pn-*H*), 5.47 (d, $^3J_{HH}$ = 3.23 Hz, 1H, Pn-*H*),5.88 (d, $^3J_{HH}$ = 2.93 Hz, 1H, Pn-*H*), 6.76 (d, $^3J_{HH}$ = 3.23 Hz, 1H, Pn-*H*), 7.29 (d, $^3J_{HH}$ = 2.93 Hz, 1H, Pn-*H*), 7.72 (d, $^3J_{HH}$ = 2.93 Hz, 1H, Pn-*H*), 7.94 (d, $^3J_{HH}$ = 2.64 Hz, 1H, Pn-*H*); $^{13}C\{^1H\}$-NMR (δC_7D_8): 8.54, 9.19, 13.62, 13.80, 14.95, 15.03, 20.70, 34.34, 38.93 (aliphatic), {87.38, 90.66, 91.93 (aromatic quaternary)}, {100.60, 100.75, 101.68,

102.50, 102.56 (aromatic *C*H)}, 103.31 (aromatic quaternary), 110.26 (aromatic CH), {119.95, 123.20, 126.00, 126.16 (aromatic quaternary)}, {126.93, 129.76 (aromatic CH)}, {131.62, 131.45 (aromatic quaternary)}, 198.27 (N*C*N); $^{29}Si\{^{1}H\}$-NMR (δC_7D_8): 0.97, 1.16, 2.25, 3.45; EI-MS: No molecular ion could be observed.

Synthesis of (**4-D**): In a similar manner as above, 18 mg (0.016 mmol) of (**3**) $0.5C_7H_8$ were dissolved in 0.5 mL of C_7D_8 and the tube attached to a Toepler line, cooled at -78 ºC and degassed before administering 5 eq of D_2 (0.73 car *ca* 9 cmHg). The tube was allowed to warm to RT and shaken well to produce (**4-D**)

Isolation of crystals of (**4**): In a N_2 filled glovebox, 50 mg (0.046 mmol) of (**3**) $0.5C_7H_8$ were placed in a 50 mL Young's ampoule and the solid dissolved with vigorous stirring a 1:1 mixture of toluene/n-pentane (*ca* 5-8 mL). The solution was freeze-thaw-degassed before being exposed to 1.5 bar of H_2. Stirring bar was removed from the solution by tying with cellotape a Nd magnet to the sides of the ampoule and the reaction mixture was placed in lagged beaker containing I.M.S. (industrial methylated spirits) cooled by solid CO_2 within a polystyrene box. Over the course of 10 days green crystals of (**4**) started appearing on the edge of the solvent. The H_2 atmosphere was carefully vented under an Ar flow and the crystals separated from the mother-liquor *via* a thin canulla before drying them under an Ar flow for *ca* 30 minutes. The mother-liquor was then placed tilted at a 45° angle and left at RT in a Young's ampoule for *ca* 3 weeks to slowly yield a second crop of (**4**). Yield: 22 mg (*ca* 46%); El. Anal.: Calcd for $C_{59}H_{106}N_2Si_4Ti_2$: C 67.39, H 10.16, N 2.66; Found C 67.90, H 10.00, N 2.53.

X-ray Crystallography: Data for (**3**) were collected at the U.K. National Crystallography Service at the University of Southampton using a Rigaku FRE+ rotating anode (Mo *Kα*) source equipped with an AFC10 four circle goniometer, Varimax HF confocal mirrors and a Rigaku HG Saturn 724+ CCD area detector operating in ω scanning mode to fill the Ewald sphere at 100K. The diffractometer was controlled using CrystalClear-SM Expert 3.1 b27, whereas integration and absorption correction were handled post data-collection using the CrysAlis Pro software. In the case of (**4**) data were collected using an Agilent Gemini Ultra diffractometer with either an Enhance Ultra (Cu *Kα*) (**4_Cu** in following table) or an Enhance (Mo *Kα*) (**4_Mo** in table below) source, equipped with an Eos CCD area detector at 173 K, operating in ω scanning mode to fill the Ewald sphere. Control, integration and absorption correction were handled by the CrysAlis Pro software. The crystals were mounted on MiTiGen loops, from dried vacuum oil kept over 4Å in an MBraun glovebox under Ar. All solutions and refinements were performed using the WinGX package and all software packages within. All non-hydrogen atoms were refined using anisotropic thermal parameters, and hydrogens were added using a riding model, except in the case of the Ti-H hydrides that were found in the difference map and refined freely. We recognize the difficulties associated with the location of hydrogen atoms next to heavy atoms as Fourier ripples can be erroneously misinterpreted for hydrogen atoms due to the sharp cut-off at high angles. Nevertheless, based on the spectroscopic evidence the hydrogen atoms have been included in the supplied models. Crystal structure, data collection and refinement details are given in the following table of this Supporting Information.

Compound	**3**	**4_Cu**	**4_Mo**
Colour, Habit	Green, Plate	Green, Plate	Green, Plate
Size/mm	0.04 x 0.05 x 0.06	0.08 x 0.1 x 0.2	0.08 x 0.1 x 0.2
Empirical Formula	$C_{59}H_{104}N_2Si_4Ti_2$	$C_{59}H_{106}N_2Si_4Ti_2$	$C_{59}H_{106}N_2Si_4Ti_2$
M	1049.6	1051.61	1051.61
Crystal System	Monoclinic	Monoclinic	Monoclinic
Space Group	*P 2₁/n*	*P 2₁/n*	*P 2₁/n*
a/Å	20.9788(8)	20.8365(8)	20.8577(16)
b/Å	13.1934(5)	13.6281(8)	13.6285(9)
c/Å	22.3687(7)	22.1659(12)	22.1312(18)
α/°	90	90	90
β/°	104.357(4)	101.286(4)	101.284(9)
γ /°	90	90	90
V/ Å³	5997.9(4)	6172.6(6)	6169.4(8)
Z	4	4	4
μ/mm^{-1}	0.383	3.201	0.372
T (K)	100	173	173
θmin/max	2.177/25.028	3.828/68.244	3.302/27.103
Completeness	99.9 to 25.028	99.5 to 68.244	99.2 to 27.103
Reflections Total/Independent	10592/6290	11249/7962	13495/5929
R_{int}	0.1678	0.0426	0.1160
Final *R1* and *wR2*	0.0612/0.1451	0.0590/0.1644	0.0911/0.1920
Goof	1.002	1.030	0.990
Larget peak hole/ e.Å^{-3}	0.356 and -0.306	0.857 and -0.771	0.561 and -0.547
ρ_{calc}/g.cm^{-3}	1.162	1.132	1.132

Selected Bond Lengths (Å) and angles (°) for (**3**): Ti(1)-Ti(2) 2.5610(8), Ti(2)-C(1) 2.300(2), Ti(2)-H(1) 1.72(3), Ti(1)-H(1) 1.79(3), Ti(1)-C(50) 2.232(4); Ti(2)-H(1)-Ti(1) 93.4(13), Ti(2)-Ti(1) -H(1) 42.0(9), C(50)-Ti(1)-Ti(2) 125.98(11), Ti(1)-Ti(2)-H(1) 44.3(9), C(1)-Ti(2)-Ti(1) 130.19(9), C(1)-Ti(2)-H(1) 86.3(9)

Selected Bond Lengths (Å) and angles (°) for (**4**): Ti(1)-C(1) 2.291(4), Ti(1)-Ti(2) 2.5413(8), Ti(1)-H(1) 1.84(5), Ti(2)-H(1) 1.79(5), Ti(2)-H(2) 1.74(4); Ti(2)-Ti(1)-H(1) 44.8(15), Ti(1)-Ti(2)-H(1) 46.4(15), H(2)-Ti(2)-H(1) 75(2), C(1)-Ti(1)-Ti(2) 132.22(9), Ti(1)-H(1)-Ti(2) 89(2)

Computational Calculations:

Density functional calculations were carried using the Amsterdam Density Functional package (version ADF2016.107).[3] The Slater-type orbital (STO) basis sets were of triple-ζ quality augmented with a one polarisation function (ADF basis TZP). Core electrons were frozen (C, N 1s; Ti 2p) in the model of the electronic configuration for each atom. The local density approximation (LDA) by Vosko, Wilk and Nusair (VWN)[4] was used together with the exchange correlation corrections of Becke and Perdew (BP86).[5,6] Local minima and transition states were confirmed by frequency calculations.

Cartesian coordinates for optimised structures.

H_2

H	-3.58553509	4.51453437	1.87556790
H	-3.12634177	3.97014110	1.63679021

$C_3N_2H_4$

C	2.80978193	-1.79969827	0.19566866
C	2.24553280	-0.56199306	0.12886667
N	0.86896338	-0.78250240	0.09108583
C	0.50349881	-2.10461869	0.12702391
N	1.74047897	-2.69506301	0.19131848
H	2.70387160	0.41996192	0.10870291
H	0.17711431	-0.04474236	0.03997879
H	1.84108570	-3.70260893	0.23190299
H	3.85056189	-2.09925670	0.24165690

$C_3N_2Me_4$

C	2.82107790	-1.80027932	0.19098747
C	2.25390034	-0.55358011	0.13495096
N	0.86836433	-0.77003372	0.09999147
C	0.51986384	-2.09616185	0.13038312
N	1.74793870	-2.70408931	0.18633620
H	3.97138290	0.72046268	0.14446748
H	-0.05740074	0.95637268	0.90276114
H	2.45394800	-4.51970100	-0.64131823
H	4.53524910	-2.84268847	-0.61373858
C	1.89267871	-4.15085871	0.22956045
H	2.40923926	-4.47060558	1.14603557
H	0.88346041	-4.57417545	0.21499188
C	4.25147353	-2.21880024	0.24855660
H	4.90713321	-1.33868725	0.24756003
H	4.47625025	-2.79695679	1.15879301
C	2.87732906	0.80176525	0.11113325
H	2.61501696	1.36030493	-0.80123728
H	2.56501629	1.41498542	0.97109298
C	-0.12730906	0.28823592	0.03202714
H	-0.01044149	0.88595596	-0.88379110
H	-1.10821419	-0.19716764	0.02616944

Ti_2Pn_2

C	4.99101510	-1.35590195	1.79684251

C	4.95474587	-1.61388027	0.34736676
C	5.02540187	-0.32459064	-0.30983968
C	5.18715428	0.67075050	0.69143058
C	5.06962204	0.08594602	1.98812133
C	5.05374370	-3.04872291	0.17433874
C	5.09686501	-2.64152285	2.47353061
C	5.23013821	-3.63485919	1.45604045
H	5.02948339	-0.14757261	-1.38377125
H	5.31096249	1.73487386	0.49638902
H	5.18914195	0.60839653	2.93186219
H	5.06397822	-3.58479051	-0.77271608
H	5.22643122	-2.80445523	3.53860656
H	5.37520825	-4.69841176	1.63906512
C	1.77621431	-1.21792645	2.71885852
C	1.01914380	-1.44712299	1.47593413
C	0.70818823	-0.14182014	0.92858326
C	1.17972782	0.84100511	1.83945701
C	1.92188609	0.22142829	2.88975582
C	0.73032224	-2.86566039	1.41667394
C	1.94247641	-2.50572854	3.37967261
C	1.21322821	-3.46316374	2.61126086
Ti	3.07464903	-2.64897297	1.39030540
H	1.05335019	1.91536994	1.71554363
H	2.36095860	0.73149778	3.74114347
H	0.17661944	-3.37818292	0.63225374
H	2.38569698	-2.68156493	4.35462125
H	1.10387514	-4.51554023	2.86852925
Ti	3.05147955	-0.31980562	0.96725060
H	0.14905158	0.05852702	0.01644436

$Ti_2Pn\dagger_2$

H	15.97117648	0.71268512	17.63075820
C	13.32796711	1.23824006	20.71869910
C	12.77843801	0.99358416	19.37459491
C	12.15511473	2.24045794	19.00037061
H	11.67005767	2.42405056	18.04354849
C	12.18723602	3.17473065	20.05770475
H	11.77759190	4.17835283	20.02882541
C	12.97804846	2.60538963	21.12240302
C	13.66583196	2.94566882	22.38184872
C	14.43897365	1.74637247	22.68027556
H	15.11095574	1.64701814	23.53149854
C	14.19992990	0.72154678	21.73996537
H	14.63000268	-0.27705630	21.77823275
C	10.36021939	2.93490628	23.57383695
H	10.48103136	4.01247424	23.60204907
C	10.65358803	2.04672201	24.62898245
H	11.06640233	2.35388037	25.58871644
C	10.40043044	0.67700319	24.24988072
C	9.81263831	0.76114002	22.90301048
C	9.75151074	2.17124591	22.51129719
C	9.02828933	2.30161707	21.23694667
C	8.65404983	0.92830642	20.91132050
H	8.06596717	0.64178576	20.04123582
C	9.16399637	0.01343800	21.85966631
H	9.05641555	-1.06768256	21.80805273
H	16.90248732	-0.33145565	18.71744870
H	15.63793877	0.73539943	19.37097109
H	15.39347974	-1.41881003	16.23081732
H	16.34361155	-2.37023314	17.38057983
C	14.87691326	-1.05536921	18.33102852
H	14.66818991	-2.83085122	17.02107082

H	14.87482941	-1.66253779	19.25703733
C	15.33518398	-1.97340238	17.17913074
C	12.30786820	-0.79320647	15.33468074
H	11.47637922	-1.45248799	15.61865128
H	13.17996447	-1.42641618	15.11464853
H	12.02277717	-0.29669079	14.39256003
Ti	10.97610804	1.22724294	20.79113245
Ti	12.12132314	1.34544910	22.87911340
Si	13.05579149	-0.44046612	18.16200915
Si	14.29271824	4.64265713	22.94622212
Si	10.47389128	-0.81678351	25.39836308
Si	7.97592763	3.73831959	20.59755901
C	11.43139924	-2.18142601	24.44010238
H	10.71579388	-2.55463384	23.68469415
C	12.61122497	-1.56235607	23.67267479
H	12.23584302	-0.89429644	22.85698961
H	13.20433800	-2.32567753	23.14156712
H	13.30354273	-1.01385836	24.32598412
C	11.87471513	-3.38916459	25.28501291
H	11.02841782	-3.85235575	25.81297936
H	12.61984520	-3.10383620	26.04228826
H	12.33511054	-4.16714054	24.65432467
C	7.87976995	-0.32227878	26.51712710
H	8.36500035	0.07163131	27.42185424
H	6.88594351	-0.69650957	26.81235903
H	7.72441578	0.52316370	25.83049792
C	8.70649416	-1.43383923	25.84204266
H	8.86046592	-2.24087984	26.58259635
C	7.92888197	-2.03708034	24.65864770
H	8.46782518	-2.87087555	24.18500109
H	7.72849526	-1.28093649	23.88600253
H	6.95380434	-2.42726240	24.99373444
C	12.83322115	0.03081661	26.90356800
H	13.04321724	0.73814372	26.08757976
H	13.41517976	-0.88309933	26.71049985
H	13.22754550	0.47184554	27.83360510
C	11.33049079	-0.27793103	27.03908748
H	10.82359675	0.67079445	27.29661016
C	11.09058582	-1.24588784	28.21553732
H	10.02263742	-1.41023525	28.41327092
H	11.53806023	-0.84576076	29.14011750
H	11.54910148	-2.22914781	28.03404599
C	15.94639346	5.69285813	25.08220753
H	16.58173176	6.14531011	24.30750070
H	16.58668109	5.49127997	25.95688810
H	15.20977042	6.45019503	25.39063369
C	15.26010055	4.40030270	24.59705573
H	16.06650649	3.69982184	24.31123933
C	14.47872092	3.73620470	25.74515521
H	13.94874956	2.83162208	25.41385538
H	13.73007447	4.41749614	26.17239669
H	15.15834468	3.44760281	26.56411058
C	16.86018817	4.37320022	21.62510933
H	17.38784541	4.38342904	22.58933768
H	17.56777615	4.73529460	20.86073062
H	16.62541627	3.32535896	21.38299286
C	15.58719852	5.23976651	21.64065302
H	15.87765437	6.25747750	21.96161822
C	15.01244052	5.34651491	20.21537049
H	14.10403691	5.96409990	20.16758718
H	14.75358448	4.35462093	19.81929349
H	15.75138393	5.79407978	19.53025416
C	12.17311767	5.99404307	24.43102563

H	11.87761564	4.99522661	24.77629080
H	11.26706579	6.62037388	24.38674728
H	12.82228355	6.42693304	25.20646339
C	12.89134672	5.97018389	23.06733863
H	12.15216797	5.66106439	22.30462849
C	13.34681080	7.40177172	22.71773101
H	13.77627528	7.47890841	21.71057141
H	14.10443734	7.76583063	23.42839768
H	12.49497643	8.09971880	22.76957286
C	9.64864445	5.72481953	19.25410694
H	10.25883619	4.88320453	18.90441675
H	10.30875531	6.60143827	19.35876296
H	8.93138306	5.95825109	18.45336938
C	8.91588230	5.42985727	20.57799406
H	9.68164478	5.33015900	21.36950805
C	8.03163678	6.64081108	20.93863942
H	7.56137254	6.54576206	21.92571723
H	7.22684867	6.78297409	20.20137064
H	8.63048620	7.56627841	20.94412939
C	8.30638290	2.82398883	17.81234141
H	9.03400125	2.09721058	18.20322694
H	8.87090959	3.69299755	17.44688636
H	7.81019357	2.36953792	16.93835266
C	7.26929466	3.22792567	18.87641385
H	6.68363463	2.31992403	19.11142641
C	6.27501812	4.26045285	18.30907772
H	5.47283221	4.50226812	19.02131760
H	5.79711961	3.88032334	17.39109013
H	6.77702219	5.20266560	18.04290188
C	6.88309703	4.09204599	23.26146947
H	7.55730514	4.94996197	23.39789458
H	7.40499104	3.20439174	23.64625026
H	6.00070434	4.26088256	23.90060926
C	6.46379459	3.88912551	21.79318524
H	5.91351169	4.79200264	21.47065107
C	5.50100988	2.69174312	21.69022563
H	5.06961775	2.58286835	20.68507215
H	4.66179358	2.80596617	22.39628912
H	6.01138159	1.74900022	21.93980573
C	11.67889144	-2.06190257	20.10609442
H	11.47141398	-1.13081813	20.67139832
H	12.60719767	-2.46675099	20.53866618
H	10.86839739	-2.76854085	20.34777195
C	11.81411340	-1.85870189	18.59001457
H	10.84450761	-1.47654178	18.21636417
C	12.06866020	-3.22759860	17.92985380
H	12.16435969	-3.16592205	16.83847871
H	11.24325053	-3.92448085	18.15062988
H	12.98928644	-3.68783360	18.31951925
C	13.63768182	1.28565670	15.89788453
H	13.85986607	2.06656519	16.63828652
H	13.26188733	1.78190457	14.98808708
H	14.58816544	0.80087563	15.62981601
C	12.61449240	0.25775594	16.41909565
H	11.66661251	0.79876202	16.60149453
C	15.89822552	0.08238285	18.52863936

$Ti_2Pn_2(C_3N_2H_4)$

C	0.84040716	1.00295401	0.71387686
C	1.23695819	0.25632343	-0.48512140
C	1.41059230	1.22763155	-1.54513765
C	1.22710455	2.52520587	-0.99419680

C	0.79134789	2.41727717	0.36602322
C	1.46146654	-1.11551043	-0.06931502
C	0.80864700	0.07465484	1.82522993
C	1.26830512	-1.17524884	1.33887296
H	1.71985830	1.02987292	-2.57097334
H	1.34963410	3.45886848	-1.54056738
H	0.63511636	3.24739186	1.04710395
H	1.83352081	-1.93348931	-0.67769897
H	0.59511394	0.31250567	2.86227683
H	1.40000045	-2.07092561	1.94429676
C	-2.43425605	1.03276170	0.86965959
C	-2.95390448	0.34429841	-0.31354376
C	-3.17377971	1.34657585	-1.33009147
C	-2.89590872	2.61820463	-0.75947021
C	-2.35228216	2.45201523	0.55478498
C	-3.20832768	-1.02760601	0.07165062
C	-2.34796218	0.06046784	1.94480839
C	-2.90979503	-1.15042698	1.45426109
C	-0.88079822	-2.07070541	-1.46073404
H	-3.01952381	3.57290687	-1.26817278
H	-2.09293602	3.25489947	1.23732368
H	-3.70036042	-1.77447387	-0.54376487
H	-2.05936199	0.25179370	2.97319636
H	-3.04357251	-2.05563700	2.04575762
Ti	-0.85696801	1.42631098	-0.82357910
Ti	-0.84224173	-0.68501141	0.29566111
H	-1.94361873	-4.69057240	-3.23607956
H	0.10440619	-3.23958617	-4.42521003
H	-2.36360930	-3.47528849	-1.01247438
N	-0.10589240	-2.06935041	-2.59984051
C	-0.40250085	-3.10136410	-3.47775170
C	-1.40799777	-3.81263163	-2.89650061
N	-1.67254177	-3.17362162	-1.68900234
H	0.58904679	-1.34833229	-2.75957736
H	-3.55496345	1.17448461	-2.33479495

$Ti_2Pn_2C_3N_2Me_4$

C	0.82074536	0.91164674	0.87218011
C	1.25605587	0.40486116	-0.43486278
C	1.50167722	1.55504466	-1.27467486
C	1.32140889	2.72415626	-0.48667012
C	0.81610540	2.36740697	0.80568754
C	1.45863619	-1.01934505	-0.28840271
C	0.72400376	-0.21979643	1.77792133
C	1.21090571	-1.35396699	1.07025625
H	1.83844376	1.53942640	-2.30962822
H	1.48480824	3.74312774	-0.83373071
H	0.63719396	3.05480168	1.62612569
H	1.83459781	-1.69782938	-1.04814516
H	0.49734293	-0.18232733	2.83857720
H	1.33400414	-2.34791055	1.49891512
C	-2.45378858	1.01854894	0.84550660
C	-2.90248401	0.55219585	-0.47237394
C	-3.05348559	1.72303777	-1.30679011
C	-2.80539221	2.87102620	-0.50611678
C	-2.34705386	2.47068990	0.79039721
C	-3.20901968	-0.85451342	-0.33938295
C	-2.45503921	-0.12256236	1.74514496
C	-3.00970433	-1.21435938	1.02025959
C	-0.90346619	-2.15326833	-1.60560824
H	-2.89222477	3.90149820	-0.84694845
H	-2.13173424	3.13827898	1.61848186

H	-3.61573040	-1.50064880	-1.11136815
H	-2.24815214	-0.10730344	2.81039227
H	-3.20986409	-2.19990387	1.43906482
Ti	-0.78177546	1.66312063	-0.63630919
Ti	-0.86732449	-0.63066502	0.10153994
H	-0.18296766	-6.17353023	-2.24969400
H	-1.77272569	-2.86515480	-5.58304521
H	-0.13442674	-4.83320513	-0.01111582
N	-0.88149054	-2.01632687	-2.97093335
C	-0.92344522	-3.24877024	-3.63577938
C	-0.97436909	-4.20643310	-2.65951199
N	-0.95991599	-3.51542112	-1.44142575
H	0.09171962	-0.65584979	-4.26236219
H	-3.37248271	1.73846225	-2.34739774
C	-0.81911128	-0.73216993	-3.65281361
H	-1.69979671	-0.58513401	-4.29312256
H	-0.80286688	0.02631597	-2.85023670
C	-0.91152355	-3.37252856	-5.12114649
H	0.00033555	-2.94064405	-5.56229345
H	-0.95316234	-4.42892818	-5.41391216
C	-1.03727344	-5.69288255	-2.75164200
H	-1.95562635	-6.09524107	-2.29597003
H	-1.02389243	-6.00834362	-3.80197337
C	-1.00099547	-4.17017087	-0.14135450
H	-0.97574966	-3.38733905	0.62777042
H	-1.92256524	-4.75813672	-0.02969884

$Ti_2Pn^{\dagger}{}_2C_3N_2Me_3$

C	9.90269658	-0.99249070	19.60184348
C	13.10927745	0.91719650	20.64213692
C	12.65292352	0.59507989	19.29206023
C	11.99594605	1.78950448	18.83713730
H	11.58045422	1.92177263	17.83956327
C	11.94151067	2.78406884	19.84402844
H	11.53847266	3.78173051	19.71821175
C	12.73216912	2.29989892	20.95787850
C	13.43555550	2.73247552	22.18372939
C	14.22596369	1.56856424	22.55527176
H	14.90887854	1.53585053	23.40203157
C	13.98944963	0.47765676	21.69048400
H	14.43867743	-0.50654291	21.79143021
C	10.53647300	2.89109376	23.53065302
H	10.83844136	3.93049760	23.51929653
C	10.70542233	1.99535122	24.60903808
H	11.19352635	2.25497435	25.54614139
C	10.20529254	0.68231089	24.28254220
C	9.57714984	0.82972087	22.96121955
C	9.78133991	2.21175301	22.50964597
C	8.99046658	2.47739195	21.29321689
C	8.29806924	1.21696023	21.07940090
H	7.58302175	1.03915155	20.27705791
C	8.67908316	0.23259535	22.01652055
H	8.32460650	-0.79407155	22.01770443
C	10.25616147	-2.81561048	21.26336426
H	10.96975892	-3.63863323	21.13360476
H	9.40131109	-3.16946747	21.85696019
H	10.74099459	-1.97950794	21.78005937
C	8.97446041	0.20849715	17.61139322
H	7.88984202	0.37145019	17.54304306
H	9.38735304	0.13238669	16.59667808
H	9.42889886	1.06074025	18.12753383
C	8.78973882	-2.25683873	18.01678295

C	8.06605090	-2.51565802	16.73887551
H	8.67432236	-2.24731616	15.86185784
H	7.12594818	-1.94600235	16.67512298
H	7.81454936	-3.57975226	16.65491032
C	8.91107120	-4.56127220	19.21644163
H	9.85812740	-5.11616524	19.30005307
H	8.36269456	-4.96773235	18.35810163
H	8.32114748	-4.77840081	20.12031978
C	9.13682956	-3.09836313	19.03736745
C	11.27208325	-2.16791508	24.72765064
H	10.58140944	-2.64254391	24.00872779
C	12.44358402	-1.58876675	23.91633970
H	12.05629613	-1.05047701	23.01027331
H	13.08987712	-2.37836285	23.49764838
H	13.08704947	-0.92342813	24.50832229
C	11.73757979	-3.27049696	25.69545961
H	10.89461042	-3.71738709	26.24274169
H	12.44784589	-2.88608709	26.44154746
H	12.24726282	-4.08416381	25.15304846
C	7.59843416	-0.21605599	26.47391271
H	8.04483421	0.29956810	27.33664140
H	6.60853961	-0.58708469	26.78680725
H	7.43865278	0.53694529	25.68819325
C	8.48140018	-1.36867518	25.95801541
H	8.63099657	-2.08131125	26.79013321
C	7.76403976	-2.13061559	24.83047363
H	8.35097775	-2.98655916	24.46559976
H	7.55335429	-1.47050943	23.97706303
H	6.79590183	-2.52480977	25.18130504
C	12.56199663	0.16451083	27.07541365
H	12.84199339	0.79659655	26.22101249
H	13.12313123	-0.77772777	26.98759228
H	12.91970480	0.66545214	27.98979893
C	11.04357848	-0.09026899	27.15430775
H	10.55478789	0.88793438	27.31601123
C	10.72440568	-0.95906824	28.38805045
H	9.64483295	-1.06443358	28.56085059
H	11.15938207	-0.50965564	29.29603146
H	11.14637717	-1.97077050	28.29563465
C	15.96873628	5.48769641	24.63886748
H	16.57113214	5.87763376	23.80604474
H	16.65692754	5.28548172	25.47650049
H	15.29442795	6.29355218	24.96550273
C	15.19091412	4.21358913	24.25292591
H	15.94448316	3.46852013	23.93867148
C	14.46776348	3.62686216	25.47917300
H	13.87449576	2.73816163	25.22027961
H	13.78526315	4.35766972	25.93411957
H	15.19279183	3.33478012	26.25733376
C	16.60132671	4.08588942	21.20585047
H	17.18615658	4.12196672	22.13575771
H	17.26611019	4.40897438	20.38744698
H	16.33786849	3.03439291	21.01745952
C	15.34489702	4.97429495	21.26684977
H	15.67058867	5.99424411	21.54332462
C	14.69360924	5.05495936	19.87374225
H	13.79001844	5.68133542	19.86103218
H	14.40121127	4.05792928	19.51648886
H	15.39795684	5.47776282	19.13789303
C	12.23764511	6.01154170	24.28883937
H	11.90922149	5.06792640	24.74201622
H	11.37759642	6.70110304	24.29116669
H	12.99527197	6.44378970	24.95890275

C	12.79958633	5.84971770	22.86113297
H	11.96580422	5.54861460	22.20159707
C	13.28917483	7.23040712	22.37561485
H	13.59477097	7.22948521	21.32200684
H	14.14586532	7.58394130	22.96917189
H	12.48912254	7.98081803	22.48835881
C	9.95250566	6.21592973	20.15591872
H	10.61787658	5.45022432	19.73861030
H	10.58452078	7.04507447	20.51300580
H	9.34642289	6.60962000	19.32664158
C	9.05828650	5.68737044	21.29255470
H	9.71948519	5.39098740	22.12617717
C	8.17756708	6.84689970	21.80375912
H	7.59809348	6.58003679	22.69646398
H	7.46597127	7.18316437	21.03406497
H	8.80463937	7.71560796	22.06375711
C	8.55568973	3.93095473	17.98623896
H	9.33339351	3.20531554	18.26212734
H	9.05154473	4.90129239	17.84720596
H	8.14122617	3.63906252	17.00654139
C	7.44729714	4.01515786	19.05116999
H	6.88135748	3.06508857	19.00990841
C	6.45913073	5.14706493	18.70772971
H	5.61338289	5.19458125	19.40809133
H	6.04306475	5.01361756	17.69510968
H	6.95680898	6.12881201	18.72316080
C	6.83924960	3.92905866	23.49106650
H	7.57174398	4.67215950	23.83854586
H	7.27240927	2.93657577	23.68090379
H	5.94119605	4.02780505	24.12345513
C	6.48289152	4.09396534	22.00128690
H	6.03755003	5.09670572	21.86758857
C	5.41311089	3.06002190	21.60687218
H	5.07089335	3.17900046	20.56863909
H	4.52680654	3.15293937	22.25704100
H	5.79329296	2.03424547	21.72209594
C	13.52000847	-2.65056685	20.14015427
H	12.94326597	-1.96241822	20.77067179
H	14.58962147	-2.46903467	20.33079009
H	13.31427740	-3.68236967	20.47330630
C	13.19085548	-2.47887713	18.64713200
H	12.10854642	-2.66110111	18.51689170
C	13.95375998	-3.55459776	17.84935915
H	13.79537367	-3.49169691	16.76587323
H	13.64174527	-4.56274632	18.17164155
H	15.03598911	-3.48744929	18.03375202
C	13.13089516	0.91797735	15.63307782
H	13.17896606	1.80868963	16.27318419
H	12.48800553	1.15949318	14.76977012
H	14.14208110	0.74315235	15.23913165
C	12.59923724	-0.32522499	16.37542932
H	11.55618954	-0.11030890	16.66813429
C	15.71546935	1.19821324	18.21838667
H	15.41049820	1.77474315	17.33290994
H	16.80633878	1.31861304	18.32362301
H	15.24026081	1.65668501	19.09479762
H	15.83307367	-0.41781386	15.93958027
H	17.19388533	-0.77530630	17.01037867
C	15.34854384	-0.29000208	18.07839397
H	15.91857679	-1.98311506	16.76464456
H	15.70942153	-0.79695350	18.99375441
C	16.10640600	-0.90867066	16.88511025
C	12.54658428	-1.52157881	15.40787904

H	12.06265473	-2.40078566	15.85527211
H	13.55192940	-1.82295475	15.07776332
H	11.97931689	-1.25617232	14.49948981
N	9.80558171	-2.30806868	19.97948843
N	9.26151795	-0.99066978	18.38427462
Si	13.44531080	-0.64525449	18.08923750
Si	14.11681644	4.44118238	22.66308435
Si	10.24760789	-0.74326775	25.51821926
Si	8.06122696	4.07795091	20.87928687
Ti	10.63392471	0.96989960	20.66285495
Ti	11.92184760	1.12445366	22.76997026

$Ti_2Pn^{\dagger}(Pn^{\dagger}\text{-}H)(\mu\text{-}H)$

Ti	11.76640421	5.77588258	9.87763737
H	12.32359838	6.87235100	11.24648137
Ti	12.98847133	5.38269135	12.02727293
Si	15.60329805	2.35677216	11.67324622
Si	13.71103468	8.17094524	8.05075742
Si	10.79288319	6.71992642	14.76571786
H	10.25926661	4.98586094	7.35833478
H	8.52486810	4.61266614	14.86837822
C	9.68658475	1.73707998	6.23755092
H	9.93497115	0.70265736	6.50635765
H	10.08942472	1.92298344	5.22855282
H	8.59182874	1.81036602	6.16062311
C	10.24085733	2.77839107	7.23185709
H	7.74485902	5.01709654	16.41163004
C	8.37417855	5.41945663	15.60119315
H	11.34403553	2.73505311	7.17285610
H	9.51706000	6.74156144	16.86354213
C	11.17640486	-0.17216249	8.78656453
H	11.83475895	-0.92300277	9.25328909
H	11.67330051	0.17527432	7.87043898
H	10.25364481	-0.69319986	8.49141722
H	7.69005940	3.43681612	11.07972165
H	6.28700500	2.41187065	10.70139525
C	10.34340939	0.40909742	11.09734851
H	11.05593620	-0.30825370	11.53633082
H	9.40031454	-0.13300024	10.93754973
H	10.15508372	1.19100093	11.84511150
C	9.80500747	8.20202924	14.03972066
C	9.66097799	6.02389795	11.15761566
H	9.20000926	6.99613258	11.29269890
C	10.52009257	5.33809504	12.08111245
C	10.93145977	4.09443209	11.45044788
C	10.27894943	3.97679189	10.14032969
C	9.46349085	5.16842323	10.05729367
H	8.80156785	5.40235320	9.22485539
C	11.78254998	3.41011850	12.40160933
H	12.22476690	2.43016213	12.27608708
C	11.78546411	4.17318818	13.60447845
H	12.27422567	3.86594656	14.52707999
C	11.09894406	5.42905115	13.41022913
C	14.95137383	6.37375369	11.15937532
H	15.23126594	7.39524678	11.40322344
C	15.30111068	5.21536089	11.90366447
H	15.92790250	5.22782253	12.79177321
C	14.73175306	4.01636673	11.31799344
C	14.07596542	4.49469889	10.09742216
C	14.26625392	5.93210619	9.97295067
C	13.72780137	6.39687832	8.70880435
C	13.22881281	5.20367929	8.07827058

H	12.77715927	5.17052486	7.08834717
C	13.34085921	4.07746859	8.93030003
H	13.04361936	3.06391115	8.68000798
C	10.60550248	9.08778929	13.06561880
H	11.09857779	8.50555312	12.27421366
H	11.38111165	9.66100608	13.59596346
H	9.94462747	9.82329982	12.57865196
H	8.49976410	9.85160837	14.62556537
C	7.42704755	0.80927028	8.78608501
H	7.50219704	2.94924516	8.61754370
H	7.80110749	6.21497163	15.10357119
H	9.84336939	9.58957266	15.74828364
C	7.93427856	2.17841515	9.28510023
C	13.56057127	7.41387157	14.38022922
H	13.77635454	6.45333980	13.85801260
H	14.53450332	7.72213447	14.79625021
H	13.26054165	8.17056877	13.64390825
C	12.51206484	7.20122953	15.48518749
C	9.11340676	9.07353216	15.10779265
C	12.47820404	8.39523611	16.45720300
H	12.20494774	9.32790319	15.94250603
H	13.46667078	8.55601502	16.91743293
H	11.75647259	8.24258377	17.27257446
C	10.43241439	4.80068355	16.93285985
H	10.65430294	3.94051599	16.28357274
H	9.79027044	4.43033373	17.74867282
H	11.37622402	5.13507439	17.38705670
C	9.72329846	5.92087053	16.15160899
H	7.78676536	-0.00851985	9.42771400
H	11.86367371	1.45252482	9.99869778
H	9.00235001	7.71156322	13.45860010
C	10.89150141	0.97541050	9.77269461
H	8.44988521	8.49208057	15.76277859
C	15.81840598	2.95739203	14.56426690
H	15.11838162	3.78595344	14.38508005
H	16.49919278	3.26277216	15.37609039
H	15.23176373	2.10828813	14.93974846
C	16.61745756	2.57823241	13.30191450
H	17.27821527	3.43295522	13.06915027
C	17.53966771	1.37679734	13.59211212
H	16.96341626	0.47394929	13.84353583
H	18.19517114	1.58924457	14.45267517
H	18.18815994	1.13034874	12.73930074
C	13.86717518	0.49865112	13.12117918
H	14.64737996	0.14566389	13.81102406
H	13.11039359	-0.29969573	13.05750897
H	13.39192030	1.37060512	13.58868676
C	14.46317028	0.79543844	11.72983261
H	13.62608171	1.02305643	11.04469266
C	15.14655247	-0.48361345	11.20267306
H	15.50239679	-0.38207221	10.16990152
H	14.44306837	-1.33182893	11.22936049
H	16.01014716	-0.76346866	11.82446571
C	16.89098820	2.12212454	10.25302821
H	17.37280571	1.14971724	10.46508738
C	17.99035402	3.20048433	10.26139771
H	17.56424680	4.20498725	10.12036801
H	18.70650589	3.03008162	9.44091814
H	18.56390786	3.20886586	11.19894616
C	16.25905339	2.03173301	8.85126617
H	15.45993277	1.27853483	8.79021390
H	17.01996138	1.76550161	8.09913150
H	15.82548207	2.99564033	8.55095092

C	15.46101319	10.47685928	7.99664664
H	15.64241134	10.41573562	6.91255751
H	16.31572422	11.01682619	8.43655578
H	14.56652037	11.09800804	8.14814243
C	15.31790941	9.07479224	8.62009385
H	15.14881891	9.21929394	9.70444451
C	16.62598308	8.27804004	8.46321300
H	16.56016913	7.27959202	8.91622905
H	17.46524396	8.81078480	8.94114392
H	16.89377881	8.14323737	7.40539394
C	14.69983052	7.49251729	5.40203377
H	15.68735122	7.89512023	5.66366979
H	14.58546310	7.58411132	4.30898175
H	14.70937586	6.41866854	5.64228261
C	13.55623668	8.22505700	6.13103316
H	13.65691891	9.30304967	5.90241344
C	12.19327493	7.77956730	5.56716872
H	12.01954129	6.70390913	5.71649960
H	12.14916136	7.96221139	4.48048720
H	11.35236394	8.31329190	6.02896979
C	11.58559669	10.20880810	8.39596811
H	12.31027093	11.03850115	8.37828774
H	10.73345748	10.53034870	9.01717282
H	11.20473091	10.08079280	7.37180495
C	12.19096393	8.90260798	8.94669443
H	12.57948440	9.12419606	9.96029096
C	11.16312305	7.76367959	9.09992477
H	10.78497676	7.44868619	8.10225273
H	10.27841879	8.14709832	9.63626011
H	7.74010627	1.69657707	11.41846747
C	7.38887016	2.45181686	10.70035280
H	10.10686685	4.34389716	5.71100046
H	12.83175828	6.31641982	16.06552672
Si	9.84232497	2.44414383	9.09776792
H	8.71729818	4.30124603	6.80388572
H	6.32542426	0.77485923	8.81317792
C	9.81129731	4.18064147	6.76026424
H	7.73821368	0.58407195	7.75836113

$Ti_2Pn^{\dagger}(Pn^{\dagger}\text{-}H)(\mu\text{-}H)(C_3N_2Me_4)$

Ti	11.97692175	5.92062738	9.88326161
H	12.63239690	7.06013382	11.15554044
Ti	13.32010290	5.61961549	12.04007524
Si	15.63006411	2.23793403	11.36935156
Si	13.89979168	8.15246989	7.84649806
Si	10.40991029	6.63860751	14.92281441
H	10.32253228	4.98551132	7.43820945
N	14.40819128	8.59443986	13.24299404
N	14.97938624	6.98258470	14.53074855
C	14.21267300	7.24516968	13.41943024
C	15.64406227	8.11429242	15.01525814
C	15.28156459	9.14272708	14.18946970
C	15.66986658	10.58447365	14.19546797
H	16.16572631	10.87893436	13.25739844
H	16.36746186	10.78735704	15.01721726
H	14.79830752	11.24419103	14.32714475
C	13.79084290	9.39863211	12.19868852
H	14.55848714	9.86527615	11.56729075
H	13.16296458	10.18380158	12.63969652
H	13.17302006	8.73032502	11.58937767
C	15.08532830	5.67800749	15.16236547
H	14.56532804	5.66681601	16.13065752

H	16.13759370	5.41077163	15.31992950
H	14.61894735	4.94693144	14.49460981
C	16.54659673	8.08455054	16.20410914
H	16.02023355	7.75248773	17.11254987
H	16.94647763	9.08678813	16.40118125
H	17.40485474	7.41037283	16.05436474
C	9.91043825	6.28331320	11.21909016
H	9.47200531	7.27020326	11.31478745
C	10.77822754	5.62420708	12.15760522
C	11.18522864	4.36764831	11.55686447
C	10.48480201	4.18993353	10.27403594
C	9.67890534	5.38831556	10.15787992
H	9.00290580	5.59625629	9.33062277
C	12.04853430	3.71243186	12.51450756
H	12.48159478	2.72674895	12.42106855
C	12.04011641	4.50092605	13.70029294
H	12.47865865	4.18754622	14.64576423
C	11.31272832	5.73143898	13.50684983
C	15.31936175	6.30837042	10.89722577
H	15.76498050	7.28219717	11.06612841
C	15.61162161	5.13505922	11.63884145
H	16.33434469	5.10634278	12.44962815
C	14.86902847	3.99261400	11.15751227
C	14.13939990	4.52204564	9.99532105
C	14.46859328	5.92416025	9.80626177
C	13.88013701	6.40763191	8.56850937
C	13.23641360	5.25277031	8.00524898
H	12.70721126	5.24063397	7.05494752
C	13.29752113	4.14555481	8.89066966
H	12.87923379	3.16540147	8.70217862
C	10.20115746	9.14630545	13.38850003
H	10.85923615	8.67395724	12.64577773
H	10.83050476	9.75903610	14.05210145
H	9.52782597	9.83691946	12.85133301
H	7.83056155	9.54191498	14.73512934
C	7.47960542	1.00481383	9.24285197
H	7.61619754	3.12280989	8.88571647
H	7.38625493	5.97690800	14.40515955
H	9.07413493	9.33678235	15.98173124
C	8.03526557	2.39848403	9.61444403
C	12.25396561	8.49185368	16.23706434
H	12.74740243	8.61430809	15.26392189
H	13.00999163	8.65722549	17.02508975
H	11.50754617	9.29577838	16.33871689
C	11.59366149	7.10904836	16.39258631
C	8.48451455	8.79818399	15.22243332
C	10.95228922	7.01754356	17.79311829
H	10.12644314	7.73829422	17.90366676
H	11.69690995	7.26154434	18.57117281
H	10.55204884	6.02057709	18.02053027
C	9.74005434	4.07253701	16.15279215
H	10.10673115	3.46463492	15.31147880
H	8.99379280	3.46775171	16.69625883
H	10.58896532	4.23652514	16.83448178
C	9.11532620	5.38698506	15.64497514
H	7.82104776	0.23716660	9.95567986
H	12.00574834	1.61237542	10.24627166
H	8.73066393	7.59040857	13.46719713
C	11.00465852	1.15642819	10.12443917
H	7.83438951	8.08562673	15.75183340
C	17.32338889	2.88668909	13.71896402
H	16.56937135	3.64982016	13.94807439
H	18.30402285	3.27169407	14.04906139

H	17.09697897	2.01024390	14.34479268
C	17.35994791	2.50826457	12.22570806
H	17.76094005	3.38024269	11.67634074
C	18.36399537	1.35227397	12.02921077
H	18.02232447	0.42684892	12.51907187
H	19.33909957	1.61196316	12.47716485
H	18.54336240	1.12155957	10.97012385
C	14.22547691	1.30588735	13.78488867
H	15.09950239	1.07291808	14.41110954
H	13.38102902	0.71271551	14.17365799
H	13.98425838	2.36655615	13.93947210
C	14.50630332	0.96720216	12.30628142
H	13.54340301	1.01805860	11.76202079
C	15.00287041	-0.49055579	12.20100670
H	15.14491616	-0.81678530	11.16157956
H	14.28200336	-1.18273359	12.66887925
H	15.96244265	-0.62406050	12.72416125
C	16.05957105	1.45160611	9.65311434
H	16.66369191	0.57366433	9.95567205
C	16.95869465	2.35294263	8.78434689
H	16.42043638	3.25914893	8.46596045
H	17.28090471	1.82060564	7.87274768
H	17.86678090	2.67692529	9.31422800
C	14.88367148	0.90848789	8.82027675
H	14.19046746	0.28974086	9.40791758
H	15.25530989	0.28629002	7.98806948
H	14.30683241	1.72782362	8.37211869
C	15.51978963	10.54767972	8.20119902
H	15.67734038	10.69559298	7.12023957
H	16.35810553	11.04748580	8.71832544
H	14.59653170	11.07978165	8.47547210
C	15.45844093	9.05000112	8.55991279
H	15.26598300	8.98501044	9.64772754
C	16.81401768	8.36643200	8.30418576
H	16.78361757	7.29060630	8.52682821
H	17.60589873	8.81746420	8.92769617
H	17.13069837	8.48086863	7.25648975
C	15.08038855	7.43313359	5.26076547
H	16.04069621	7.88431835	5.54572885
H	15.00913446	7.47422040	4.15958493
H	15.11784397	6.37038531	5.54851783
C	13.87590363	8.14434683	5.91034193
H	13.93991772	9.22012979	5.64878331
C	12.56677667	7.61185194	5.28864986
H	12.48742274	6.51988687	5.39991110
H	12.54112139	7.82136817	4.20549432
H	11.66714909	8.05540684	5.73709543
C	11.70667541	10.16372910	7.86504884
H	12.42461141	10.98932692	7.72361984
H	10.85055223	10.56441237	8.43508204
H	11.32621605	9.88758206	6.86922535
C	12.32366308	8.95195470	8.59743972
H	12.67955561	9.32615157	9.57791042
C	11.31969259	7.81370814	8.88821912
H	10.95099648	7.39019065	7.92750803
H	10.42407996	8.24012605	9.37508755
H	7.85236969	2.10716281	11.78461736
C	7.51187648	2.80712614	11.00568683
H	10.08757690	4.24384137	5.84096795
H	12.39606718	6.34740690	16.34673248
Si	9.95726620	2.59766864	9.36897887
H	8.74984414	4.28450621	7.00031914
H	6.37626496	1.00840451	9.28294637

C	9.84065797	4.15003538	6.91250605
H	7.77091323	0.67447549	8.23686682
C	9.39364260	8.10665861	14.18635254
H	7.23898881	4.37192550	15.14810606
H	8.31490049	4.60926032	13.75520873
C	9.66134252	1.67382000	6.56846044
H	9.91199464	0.65760261	6.90037880
H	10.01343805	1.77906520	5.52796937
H	8.56427177	1.75621987	6.54205329
C	10.27925600	2.77510310	7.45648104
C	7.95197591	5.07570595	14.68433145
H	11.37626667	2.71000585	7.33634927
H	8.69299546	5.91436087	16.52314310
C	11.18252790	-0.09046871	9.23641056
H	11.81666033	-0.83844942	9.74299403
H	11.66046858	0.14326181	8.27443960
H	10.21900289	-0.57960590	9.02362504
H	7.84260908	3.81417676	11.29673087
H	6.40792713	2.79606575	11.02056293
C	10.51582348	0.74222157	11.52771294
H	11.23666072	0.05630223	12.00524011
H	9.55433020	0.20938026	11.47107310
H	10.38027824	1.60284862	12.19612673

$Ti_2Pn^{\dagger}{}_2H(\mu\text{-}H)C_3N_2Me_4$

C	10.02605959	-1.03762131	19.56713534
C	13.28736598	1.05985639	20.54171280
C	12.76327303	0.64600947	19.24706023
C	11.96981642	1.76784303	18.81213487
H	11.49471136	1.84803964	17.83714028
C	11.89744205	2.77445496	19.81327097
H	11.39899400	3.72803922	19.70133390
C	12.79832854	2.38699021	20.87850166
C	13.48450195	2.86629130	22.08917854
C	14.36425695	1.76870181	22.43528635
H	15.05356439	1.77244901	23.27604265
C	14.19823438	0.65958434	21.57933861
H	14.72911159	-0.28059874	21.66503160
C	10.66386524	2.78059054	23.55888691
H	10.96173483	3.81993171	23.56396329
C	10.85898446	1.85171039	24.61293469
H	11.38469491	2.08130140	25.53888990
C	10.33345422	0.55014602	24.27958868
C	9.67375476	0.75537870	22.99522702
C	9.87096194	2.12602299	22.55437715
C	9.09035987	2.38373338	21.33357629
C	8.43301723	1.11523604	21.08362470
H	7.70878965	0.94178981	20.29024742
C	8.84051746	0.12293555	22.00963792
H	8.50274996	-0.90864839	22.01016938
C	10.64336500	-2.91915085	21.11297521
H	11.39065056	-3.67678275	20.84693897
H	9.87803999	-3.37873821	21.75237597
H	11.12727828	-2.10034116	21.65445258
C	8.91506638	0.16076576	17.67029952
H	7.82203675	0.25585964	17.61066162
H	9.32634502	0.14217137	16.65194137
H	9.31892988	1.02366758	18.20654745
C	8.85015808	-2.31478345	18.03887301
C	8.03644170	-2.57604282	16.81424375
H	8.56447295	-2.27132898	15.89725749
H	7.07438495	-2.03984576	16.83491841

H	7.81468355	-3.64685771	16.72764756
C	9.18829072	-4.64251156	19.15282916
H	10.16645792	-5.14765009	19.14552717
H	8.59415845	-5.05613999	18.32873070
H	8.68629547	-4.91380634	20.09453897
C	9.32477660	-3.16324590	19.00160205
C	10.14615907	-2.58550404	24.84612834
H	9.59788358	-2.47199203	23.89022448
C	11.56383019	-3.08867661	24.51081284
H	12.14038380	-2.34445102	23.94072752
H	11.52002846	-4.02829395	23.93075876
H	12.12713883	-3.31148826	25.43132917
C	9.39539358	-3.64373197	25.68150565
H	8.34463636	-3.37883357	25.86554393
H	9.87423342	-3.79390791	26.66201148
H	9.40608061	-4.62115172	25.16787615
C	8.10785660	0.80556373	26.99972627
H	8.80016420	0.93668764	27.84495533
H	7.08262198	0.91202419	27.39499251
H	8.27754203	1.63748223	26.29797350
C	8.29027732	-0.55509585	26.30040057
H	8.16536572	-1.34528085	27.06624109
C	7.19273297	-0.75719031	25.23773159
H	7.25966542	-1.73925604	24.74479379
H	7.25726075	0.01125240	24.45218993
H	6.18778602	-0.68366984	25.68880152
C	12.80231230	-0.47142405	26.68774425
H	13.02829857	0.03825739	25.73977380
H	13.14473632	-1.51169550	26.57536856
H	13.40816772	-0.01307462	27.48874849
C	11.30259940	-0.41655061	27.04126684
H	11.06240219	0.63713791	27.28248762
C	11.01931994	-1.23907217	28.31544134
H	9.97356301	-1.15778924	28.64753137
H	11.65848754	-0.90142202	29.14954652
H	11.23570858	-2.30784105	28.15772810
C	16.04217973	5.68177356	24.44662031
H	16.50806096	6.17280559	23.57966390
H	16.83975273	5.48973517	25.18495318
H	15.34850419	6.40465438	24.90392901
C	15.32389651	4.37042502	24.06389894
H	16.08839796	3.70971617	23.61517444
C	14.79841444	3.66225560	25.32871721
H	14.24148544	2.74225544	25.09998722
H	14.12825209	4.31631046	25.90557608
H	15.63326666	3.38751419	25.99630617
C	16.36274451	4.58673593	20.85306307
H	17.04568573	4.57303095	21.71549828
H	16.90923587	5.04206263	20.00895817
H	16.14887133	3.54202151	20.57889676
C	15.06412644	5.36446848	21.14389680
H	15.35093217	6.37699392	21.48914409
C	14.24814510	5.53060869	19.84677616
H	13.30737514	6.08001749	20.00237530
H	13.98898570	4.55137404	19.41727106
H	14.82945569	6.08120133	19.08695553
C	12.19356448	5.84896293	24.54773247
H	11.98863782	4.83898500	24.92474604
H	11.27666721	6.44698848	24.68464696
H	12.96237042	6.28727990	25.20249845
C	12.65147108	5.88162559	23.07314815
H	11.79230405	5.58444213	22.44451916
C	12.99460891	7.34257788	22.70792889

H	13.21564448	7.47689169	21.64092346
H	13.86758245	7.70345451	23.27406537
H	12.15166739	8.00903904	22.95913417
C	10.04190403	6.15411285	20.31825224
H	10.77526952	5.41742067	19.96881628
H	10.60818606	7.01045917	20.72083412
H	9.49460073	6.51909208	19.43529389
C	9.07584055	5.59840774	21.38237317
H	9.67900057	5.30260838	22.26011479
C	8.14610744	6.74513803	21.83745087
H	7.51027579	6.46906757	22.68890578
H	7.48357301	7.07565709	21.02147088
H	8.74364054	7.62152840	22.14081152
C	8.69174018	3.86449584	18.00337954
H	9.48989727	3.15723239	18.26804667
H	9.15926436	4.85487301	17.90057165
H	8.30562995	3.58700095	17.00698959
C	7.56142977	3.88187434	19.05014016
H	7.05172006	2.89980982	18.99651113
C	6.51571081	4.95438359	18.68073962
H	5.65159070	4.95203868	19.36035976
H	6.13306574	4.79735602	17.65733793
H	6.95455176	5.96454736	18.70801899
C	6.78393880	3.83676061	23.47711775
H	7.47439864	4.61411595	23.83739879
H	7.23527836	2.86339500	23.72409082
H	5.85062326	3.92779677	24.05912991
C	6.50161104	3.94424965	21.96544730
H	6.03046672	4.92895527	21.77782583
C	5.48511363	2.86386491	21.54752315
H	5.19675500	2.93745693	20.48777199
H	4.56101297	2.94943326	22.14513505
H	5.88861237	1.85386782	21.71837664
C	13.96753674	-2.50522606	20.15679235
H	13.39728677	-1.85446008	20.83099170
H	15.03202853	-2.23274100	20.24199413
H	13.87989819	-3.54026217	20.53139810
C	13.48932640	-2.40905040	18.69482690
H	12.40983375	-2.65288503	18.67516045
C	14.22644166	-3.48036079	17.86301373
H	13.97524964	-3.45751170	16.79445688
H	13.98281147	-4.48921706	18.23968702
H	15.31779811	-3.36793915	17.95194374
C	12.89709494	0.87461943	15.58041226
H	12.94301870	1.78143264	16.19803153
H	12.15343895	1.04755324	14.78256067
H	13.87567923	0.76772646	15.08781258
C	12.54416044	-0.38875353	16.39267422
H	11.51840080	-0.25596907	16.78342733
C	15.69984422	1.43734433	17.86268133
H	15.32076289	1.90719094	16.94164006
H	16.78393657	1.63979445	17.90625332
H	15.22849925	1.94523926	18.71585243
H	15.79712295	-0.36472265	15.71984469
H	17.25010573	-0.50983208	16.72194900
C	15.43639311	-0.08096551	17.87106937
H	16.07288251	-1.83770634	16.67021616
H	15.88565258	-0.48012718	18.80256126
C	16.17169302	-0.74359585	16.68465886
C	12.50019338	-1.61044693	15.45522189
H	12.12175345	-2.51017070	15.96078015
H	13.49470143	-1.84707648	15.04550545
H	11.83907900	-1.41204586	14.59281272

N	10.03023853	-2.36609701	19.91250415
N	9.28454699	-1.03649431	18.40742765
Si	13.56797192	-0.58799509	18.03392865
Si	14.05467684	4.61224596	22.61747572
Si	10.07817595	-0.79703485	25.59039756
Si	8.12540644	3.97007950	20.90366549
Ti	10.74423211	0.87370638	20.63923212
Ti	12.11982424	1.06446607	22.76139165
H	12.70013335	-0.41538563	23.46799139
H	11.56798345	-0.31724167	21.72150629

$Ti_2Pn(C_8H_5Si^iPr_3\text{-}H)(\mu\text{-}H)(C_3N_2H_4)$

Ti	11.90207670	5.77742265	9.95198794
H	12.70146854	7.01332648	11.02137160
Ti	13.42484029	5.66388417	11.98350824
C	12.22155036	8.71360645	8.45440670
Si	13.65686602	7.81575386	7.55850713
H	10.42161939	8.15720548	9.52343234
H	12.72735796	9.11549381	9.35481057
N	13.94419809	8.76923324	13.18768552
N	15.15400284	7.33688373	14.22755215
C	14.22906821	7.42619189	13.21223906
C	15.44503670	8.57711554	14.80386685
C	14.67216737	9.49199863	14.14194728
H	14.85441000	11.52156830	13.41982174
H	11.82263736	6.12756517	5.44636853
H	11.79555289	7.34693152	4.16771908
H	11.15276471	7.73243238	5.77980413
H	12.90563458	10.45204721	12.50354838
C	13.36076441	7.68300478	5.65757271
H	13.44646498	8.73445570	5.32197975
C	11.95394033	7.20153774	5.24935868
H	16.81850852	6.06217595	14.51462050
H	10.80370668	10.37769871	8.39775047
H	11.05111150	9.61483585	6.82211680
H	14.73422316	2.94053209	11.54123679
H	17.43240465	8.40027830	15.62891815
C	11.56533480	9.91768857	7.74601549
H	10.68912121	7.20304633	8.06877204
H	12.28883590	10.70473241	7.47677382
C	9.94850876	6.16160213	11.35196159
H	9.44005698	7.11960369	11.35949968
C	10.92439902	5.69279454	12.29955911
C	11.32913006	4.35729858	11.89614832
C	10.57061408	4.00336010	10.71860135
C	9.67911337	5.08864097	10.46293249
H	8.94111010	5.11613926	9.66271255
C	12.25548160	3.85662395	12.88997851
H	12.66260351	2.85245863	12.94444033
C	12.33626721	4.84442901	13.91730885
H	12.86855278	4.73182130	14.85959848
C	11.61063173	6.00930722	13.52134142
C	15.34656318	6.12763405	10.60748661
H	15.87105411	7.07691317	10.64539658
C	15.62384089	4.99633298	11.42909882
H	16.41316629	4.94584431	12.17526745
C	14.71506935	3.93902835	11.11697876
C	13.96380016	4.36727863	9.95824751
C	14.37004906	5.72189490	9.62591641
C	13.69477694	6.13115456	8.40428667
C	12.95821288	4.97164094	7.98694473
H	12.36392963	4.91438752	7.07706351

C	13.03724003	3.92882620	8.94796016
H	12.59743710	2.94120743	8.85264219
C	11.21365873	7.65106720	8.94196637
C	15.39924683	10.12149923	7.27545491
H	15.43993931	10.04642469	6.17771653
H	16.31007700	10.65511635	7.59514126
H	14.53829408	10.75526293	7.53208200
C	15.31710595	8.72923395	7.92926639
H	15.26096509	8.88722118	9.02399350
C	16.60069097	7.92451822	7.65298880
H	16.56226004	6.91735011	8.09009018
H	17.48247178	8.44076903	8.06930527
H	16.78030357	7.81011827	6.57428600
C	14.43261563	6.86942643	4.90822585
H	15.44147315	7.27986536	5.04534728
H	14.22554599	6.85685950	3.82472908
H	14.45369036	5.82395389	5.25130944
H	10.55256628	3.03921394	10.22243359
H	11.50687874	6.91630398	14.10867181
C	14.56884909	10.96905139	14.32784254
H	13.55004202	11.28200100	14.60338548
H	15.23953824	11.29086485	15.13392680
C	12.96554420	9.38018078	12.29167150
H	13.25615692	9.22677760	11.24720614
H	11.98122184	8.92210029	12.43593451
C	16.42703833	8.74785310	15.91317713
H	16.50915620	9.80635754	16.18757116
H	16.13006839	8.19366903	16.81716793
C	15.73677292	6.09187569	14.70689003
H	15.56421443	5.98079234	15.78602440
H	15.25000952	5.26875719	14.17303815

$Ti_2Pn(C_8H_5Si^iPr_3)H(\mu\text{-}H)(C_3N_2H_4)$

C	10.14203721	-1.20875775	19.76469769
C	13.19764339	1.00124025	20.55345420
C	12.62017313	0.45287722	19.35474704
C	11.80690637	1.46658437	18.76955499
H	11.31937013	1.39206700	17.79951424
C	11.71869093	2.58550957	19.65215480
H	11.21934029	3.52453092	19.43684817
C	12.63640013	2.32877490	20.74375096
C	13.28724458	2.91986715	21.88978189
C	14.26426137	1.98180641	22.33955043
H	14.95080226	2.14292401	23.16881125
C	14.15533719	0.76867715	21.60452064
H	14.75876352	-0.11976354	21.75444571
C	10.76451296	2.85545218	23.61578793
H	11.08929017	3.89092111	23.62406345
C	10.92051897	1.92448134	24.67887978
H	11.45711733	2.13878220	25.60231741
C	10.33354583	0.64970190	24.36322556
C	9.66544061	0.86443101	23.08368221
C	9.93777404	2.21623642	22.62367657
C	9.18977921	2.44386436	21.40381439
C	8.40807355	1.26830860	21.18197516
H	7.65486348	1.15093642	20.40601065
C	8.77064076	0.26417078	22.12424812
H	8.35314079	-0.73691634	22.16676872
H	11.24557988	-5.13138476	19.06282594
H	8.99952805	0.69528801	18.45835936
C	10.97783586	-1.33280159	28.32520458
H	9.93148356	-1.26071414	28.65510064

Si	10.05523678	-0.70514820	25.65505475
H	11.61447743	-1.06308310	29.18417980
Ti	10.68463210	0.79988116	20.74552198
H	12.84551741	-0.51189188	18.91152724
C	9.18067874	-2.67307956	18.25669626
N	10.50982764	-2.50643339	20.02020443
H	11.51766247	-0.31164230	21.88737345
H	11.18237229	-2.38949247	28.09407932
H	12.74500809	-0.32381770	23.53311526
H	9.08053030	3.38863801	20.88145582
H	8.38642590	-4.17271984	16.96353288
N	9.32189400	-1.34250542	18.66712824
Ti	12.11134185	1.11731889	22.79495686
C	9.93928884	-3.41388601	19.12061836
C	10.11600631	-2.47501329	24.88665004
H	9.66401965	-2.34299745	23.88535005
C	11.54699532	-3.00525933	24.68127779
H	12.18339157	-2.27603357	24.15953543
H	11.53663159	-3.94524875	24.10287821
H	12.02075034	-3.23609661	25.64724436
C	9.27425023	-3.51982907	25.64600212
H	8.21973208	-3.22930319	25.74598741
H	9.66650437	-3.69077972	26.65977922
H	9.30260705	-4.49144602	25.12420176
C	8.15654202	0.91767157	27.12039756
H	8.84362517	0.98185776	27.97630498
H	7.13381363	1.05546910	27.50924979
H	8.37131595	1.76793575	26.45497390
C	8.28033842	-0.42000230	26.36756907
H	8.11554126	-1.23387419	27.09741691
C	7.17850894	-0.52226148	25.29659408
H	7.20620118	-1.47783208	24.75212956
H	7.27414803	0.28266102	24.55382969
H	6.17865053	-0.43235919	25.75352566
C	12.78307313	-0.47752965	26.77195083
H	13.02632304	0.08830985	25.86192952
H	13.11667456	-1.51014701	26.59829528
H	13.38322045	-0.07833592	27.60685650
C	11.28242735	-0.42627517	27.11586933
H	11.05750814	0.61090662	27.42890518
H	13.16876665	3.93553311	22.25140318
H	12.32653666	-3.37582864	20.64940541
C	8.34429467	-3.08459517	17.09337244
H	7.28702260	-2.80724353	17.22585218
H	8.69013159	-2.62607102	16.15378079
C	8.67580358	-0.23438397	17.97820210
H	8.96683679	-0.21669506	16.91894464
H	7.58199162	-0.31604327	18.04497717
C	10.18014460	-4.88372032	19.18675010
H	9.85470848	-5.30943179	20.14826145
H	9.62452180	-5.39589313	18.39195393
C	11.41891248	-2.93014626	21.08029843
H	11.68857199	-2.04872950	21.67207349
H	10.92861626	-3.67159458	21.72391576

Transition state

C	10.20093800	-1.04782200	20.10401700
C	13.01584600	1.02334100	20.35182300
C	12.34528900	0.65579200	19.12585100
C	11.61813800	1.79144800	18.67539800
H	11.04980000	1.84032900	17.74746500
C	11.68458500	2.83424400	19.64184100

H	11.25644900	3.82531400	19.53408300
C	12.61223000	2.39660200	20.67017800
C	13.42176200	2.84987600	21.79289600
C	14.36150800	1.80395900	22.06896200
H	15.15173400	1.85713200	22.81649500
C	14.06945000	0.66875200	21.26782800
H	14.59710500	-0.28139100	21.30087200
C	10.98747600	2.79870500	23.72415000
H	11.35256700	3.81329200	23.84745500
C	11.10309200	1.75100500	24.68385700
H	11.65796300	1.83983800	25.61704700
C	10.44011900	0.55543800	24.24492600
C	9.76681300	0.91598700	22.99520700
C	10.09318900	2.31277800	22.68552300
C	9.26149600	2.73755600	21.57396200
C	8.38178900	1.65683000	21.28431700
H	7.59339900	1.67933900	20.53277100
C	8.72766300	0.52212800	22.06746700
H	8.22079300	-0.43731600	22.03367000
H	10.38802800	-4.36096800	20.27897200
H	8.95583800	-0.84600500	18.43474800
C	10.76712300	-1.88479300	28.01210800
H	9.70554600	-1.82732000	28.29079000
Si	9.98608300	-0.86251600	25.40890100
H	11.35815200	-1.73743600	28.93114100
Ti	10.62777900	1.06047000	20.73063600
H	12.46041500	-0.27839200	18.58452700
C	9.38117800	-2.87586400	18.96179900
N	10.62620700	-2.22349100	20.65036400
H	13.91190200	-1.26823500	23.82200600
H	10.96517500	-2.91038300	27.66554100
H	13.99602800	-0.52582100	23.70461700
H	9.19935500	3.73640200	21.15494400
H	8.82073100	-3.39889800	18.19627200
N	9.43002400	-1.48898300	19.05975700
Ti	12.14272000	1.16835200	22.62022100
C	10.15023200	-3.34667400	19.98268400
C	9.93365600	-2.53656300	24.44906900
H	9.36174800	-2.28037700	23.53725900
C	11.31677000	-3.03270800	23.99524900
H	11.88790800	-2.24395000	23.47956000
H	11.22906000	-3.90113200	23.31875200
H	11.92831700	-3.36121200	24.84846700
C	9.17243500	-3.66802400	25.16578400
H	8.15303000	-3.37204000	25.44823600
H	9.68936200	-3.98558500	26.08296300
H	9.09034200	-4.55649500	24.51725000
C	8.13363600	0.78666400	26.89037600
H	8.81554100	0.79842400	27.75271900
H	7.11401400	0.94836700	27.27709500
H	8.38577400	1.64735300	26.25300300
C	8.21222900	-0.53151700	26.09720700
H	8.01935500	-1.36055000	26.80378900
C	7.10787100	-0.56900400	25.02536000
H	7.10509600	-1.50906800	24.45407300
H	7.22493100	0.25474300	24.30776100
H	6.11324900	-0.46451500	25.48985700
C	12.66685200	-0.91871800	26.65664600
H	12.99074000	-0.15813900	25.93420200
H	12.95731500	-1.90037500	26.25460800
H	13.24417300	-0.76852600	27.58417000
C	11.15752200	-0.84473400	26.94285900
H	10.96521000	0.15283500	27.38020400

H	13.45469000	3.85260900	22.20605100
H	11.21574400	-2.22603500	21.47979900

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