
Supplementary information

**Hydroamination of alkenes with dinitrogen
and titanium polyhydrides**

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Supplementary Information for

**Hydroamination of alkenes with dinitrogen and
titanium polyhydrides**

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1. General information

All reactions were carried out under a dry and oxygen free argon atmosphere by using Schlenk techniques or under a nitrogen or argon atmosphere in an Mbraun glovebox. The argon was purified by being passed through a Dryclean column (4A molecular sieves, Nikka Seiko Co.) and a Gasclean GC-XR column (Nikka Seiko Co.). The nitrogen and the argon in the glovebox were constantly circulated through a copper/molecular sieves catalyst unit. The oxygen and moisture concentrations in the glovebox atmosphere were monitored by an O₂/H₂O Combi-Analyzer (Mbraun) to ensure both were always below 1 ppm. Samples for NMR spectroscopic measurements were prepared by using Schlenk techniques or in the glovebox by use of J. Young valve NMR tubes. ¹H, ¹³C, and ¹⁵N NMR spectra were recorded on a JEOL JNM-ECS400 or Bruker-AVANCE500HD spectrometer. Evans NMR spectroscopy was performed by measuring the shift in frequency for the ¹H NMR signal of cyclohexane in a capillary containing 1 mol % cyclohexane in benzene-*d*₆ relative to a 1 mol % cyclohexane in benzene-*d*₆ solution containing the desired paramagnetic compound¹. IR spectra were recorded by Nujol mull and KBr pellet on Jasco FT/IR-4X spectrometer. Elemental analyses were performed by a J-SCIENCE MICRO CORDER JM10 or YANACO CHN CORDER MT-6. High-resolution MS were recorded on a JEOL JMS-700V (EI). Field desorption (FD) mass spectra were acquired on a JEOL JMS-T100GCV time of flight mass spectrometer equipped with an EI/FI(FD) combination ion source. ESR (electron spin resonance) spectra were recorded on a JEOL JES-RE3X spectrometer. Anhydrous THF, hexane, benzene, Et₂O, and toluene were purified by use of a SPS-800 solvent purification system (Mbraun), and dried over fresh Na chips or activated molecular sieves in the glovebox. NMR solvents were dried with activated 3A molecular sieves. $[(C_5Me_4SiMe_3)Ti]_3(\mu_3-H)(\mu-H)_6$ (**1**) (ref. 2), $[(C_5Me_4SiMe_3)Ti]_3(\mu_3-N)(\mu-NH)(\mu-H)_2$ (**2**) (ref. 2), $[(C_5Me_4SiMe_3)Ti]_3(\mu_3-^{15}N)(\mu-^{15}NH)(\mu-H)_2$ (**2-¹⁵N**) (ref. 2), TiCl₃(THF)₃ (ref. 3), and [C₅Me₄SiMe₂^{*t*}Bu]Li (Cp^{*+*}Li) (ref. 4) were prepared according to literature procedures. ¹⁵N₂ (99.9%), D₂ (99.96%) were purchased from SHOKO science. Hydrogen (>99.99999%) was purchased from TAIYO NIPPON SANSO and used as received. Other chemicals were purchased from common commercial sources and used as received.

2. Experimental details

Preparation of [Cp''TiCl₃]: THF solution (35 mL) of [C₅Me₄SiMe₂^tBu]Li (Cp''Li) (1.68 g, 6.94 mmol) was slowly added to a suspension of TiCl₃(THF)₃ (2.57 g, 6.94 mmol) in THF (35 mL) at room temperature. The mixture was refluxed for 1 day. The color of the solution changed from pale blue to deep green. After the reaction, the solution was cooled to 0 °C and treated dropwise 2 mL of conc. HCl. After removal of the solvent under vacuum, the residual solid was extracted with toluene and filtered. Then the solution was evaporated. The residue was recrystallized from toluene at –30 °C to afford [Cp''TiCl₃] (1.52 g, 3.91 mmol, 56%) as red needle crystals.

Characterization of [Cp''TiCl₃]: ¹H NMR (C₆D₆, rt): δ 2.29 (s, 6H, C₅Me₄Si^tBuMe₂), 1.92 (s, 6H, C₅Me₄Si^tBuMe₂), 0.69 (s, 9H, C₅Me₄Si^tBuMe₂), 0.53 (s, 6H, C₅Me₄Si^tBuMe₂). ¹³C{¹H} NMR (C₆D₆, rt): δ 144.5 (s, C₅Me₄Si^tBuMe₂), 142.3 (s, C₅Me₄Si^tBuMe₂), 138.4 (s, C₅Me₄Si^tBuMe₂), 27.2 (s, C₅Me₄Si^tBuMe₂), 20.3 (s, C₅Me₄Si^tBuMe₂), 18.0 (s, C₅Me₄Si^tBuMe₂), 14.0 (s, C₅Me₄Si^tBuMe₂), –2.1 (s, C₅Me₄Si^tBuMe₂). Anal. calcd. for C₁₅H₂₇Cl₃SiTi: C, 46.23; H, 6.98. Found: C, 46.82; H, 6.90.

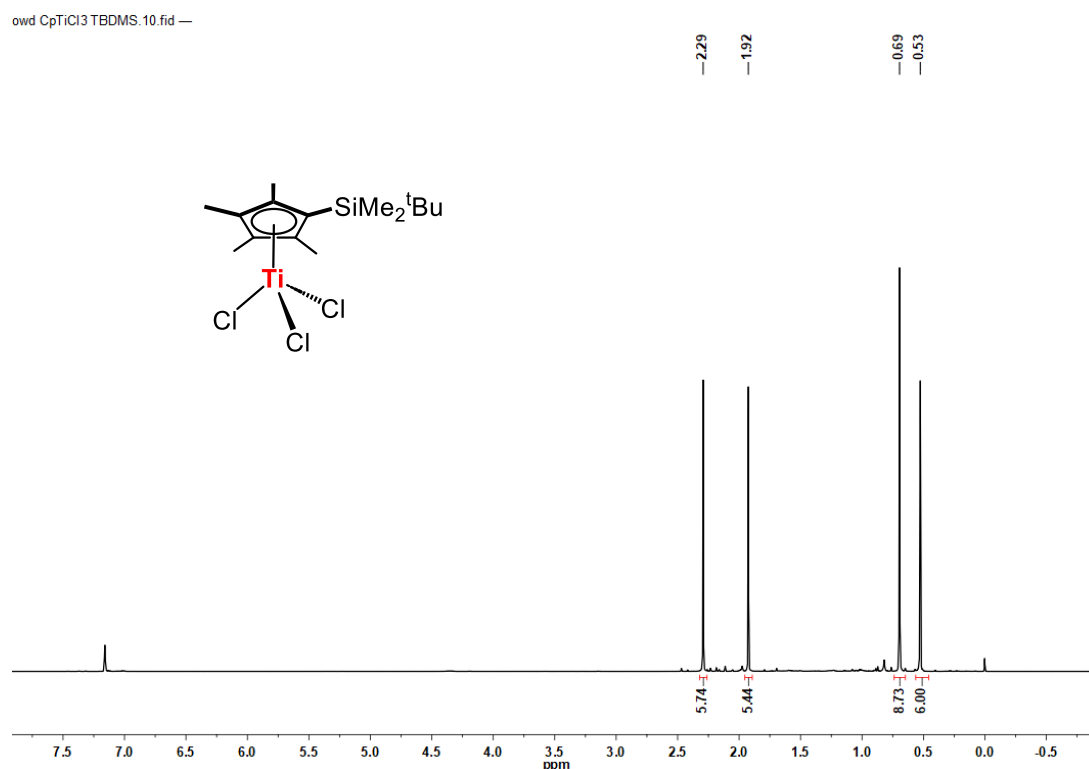


Figure S1. ¹H NMR spectrum of [Cp''TiCl₃] (C₆D₆, rt).

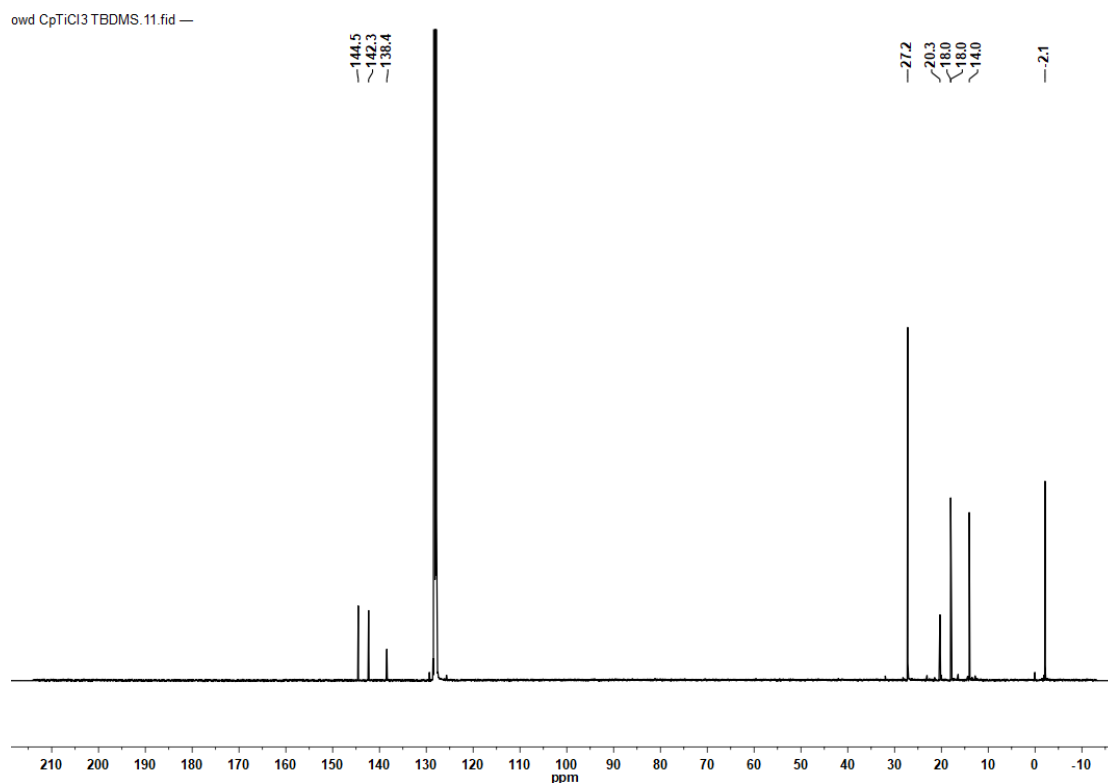


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Cp}''\text{TiCl}_3]$ (C_6D_6 , rt).

Preparation of $[\text{Cp}''\text{Ti}(\text{CH}_2\text{SiMe}_3)_3]$: Toluene suspension (14 mL) of $\text{LiCH}_2\text{SiMe}_3$ (249 mg, 2.64 mmol, 3 equiv.) was slowly added to a solution of $[\text{Cp}''\text{TiCl}_3]$ (343 mg, 0.879 mmol) in toluene (10 mL) at room temperature. The mixture was stirred for 1 h. After removal of the solvent under vacuum, the residue was extracted with hexane and filtered. The hexane solution was concentrated and recrystallized at $-30\text{ }^\circ\text{C}$ to give $[\text{Cp}''\text{Ti}(\text{CH}_2\text{SiMe}_3)_3]$ (465 mg, 0.853 mmol, 97%) as yellowish-brown block crystals.

Characterization of $[\text{Cp}''\text{Ti}(\text{CH}_2\text{SiMe}_3)_3]$: ^1H NMR (C_6D_6 , rt): δ 2.11 (s, 6H, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 1.88 (s, 6H, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 1.55 (s, 6H, $\text{Ti}(\text{CH}_2\text{SiMe}_3)_3$), 0.91 (s, 9H, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 0.35 (s, 6H, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 0.28 (s, 27H, $\text{Ti}(\text{CH}_2\text{SiMe}_3)_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , rt): δ 129.6 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 127.8 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 119.7 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 86.1 (s, $\text{Ti}(\text{CH}_2\text{SiMe}_3)_3$), 27.5 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 20.7 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 16.6 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 13.3 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 3.0 (s, $\text{Ti}(\text{CH}_2\text{SiMe}_3)_3$), -1.7 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$). Anal. calcd. for $\text{C}_{27}\text{H}_{60}\text{Si}_4\text{Ti}$: C, 59.51; H, 11.10. Found: C, 59.99; H, 10.71.

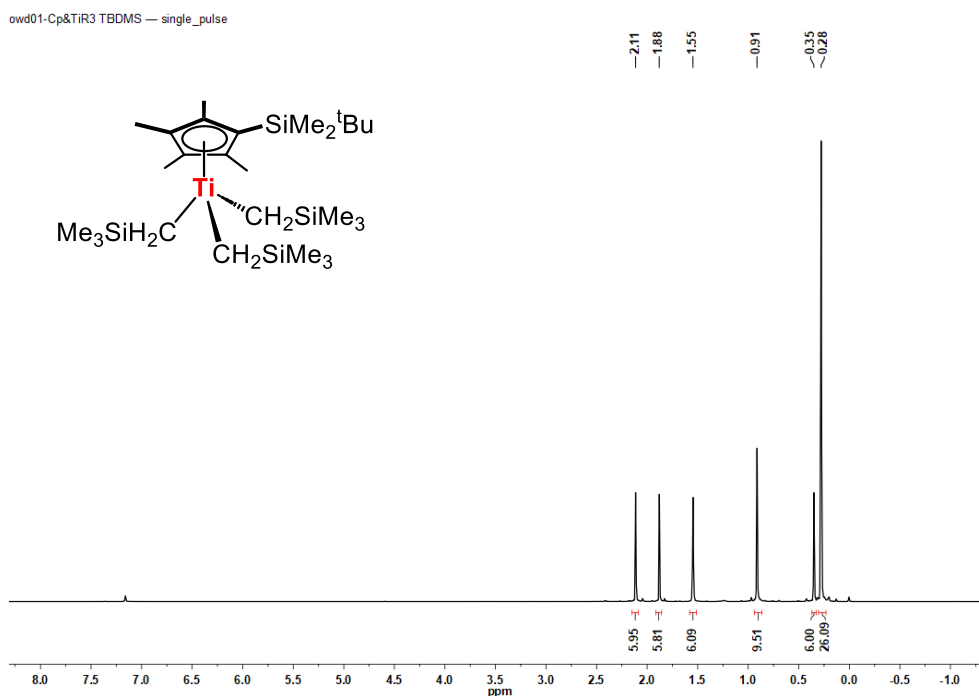


Figure S3. ^1H NMR spectrum of $[\text{Cp}''\text{Ti}(\text{CH}_2\text{SiMe}_3)_3]$ (C_6D_6 , rt).

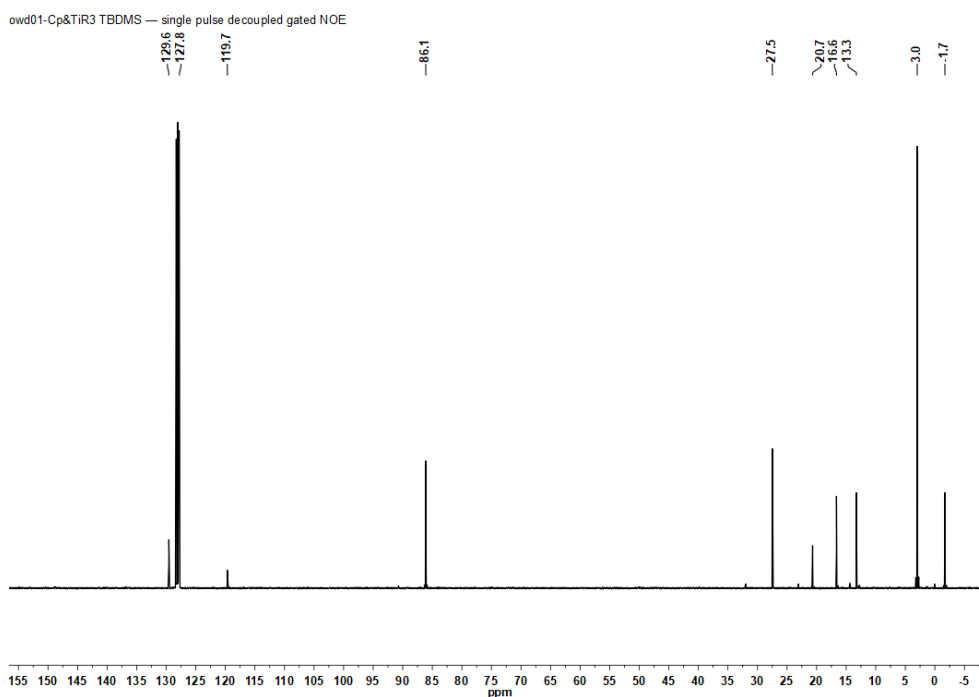


Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $[\text{Cp}''\text{Ti}(\text{CH}_2\text{SiMe}_3)_3]$ (C_6D_6 , rt).

Preparation of $[(\text{Cp}''\text{Ti})_3(\mu_3\text{-H})(\mu\text{-H})_6]$ (1'**):** A hexane solution (6 mL) of $[\text{Cp}''\text{Ti}(\text{CH}_2\text{SiMe}_3)_3]$ (626 mg, 1.15 mmol) in 10 mL Hiper Glass Cylinder (TAIATSU TECHNO[®]) was filled with H_2 (4 atm). The solution was stirred at 60 °C for 19 h. After the reaction, the solution was evaporated and recrystallized in hexane solution at −30 °C to give **1'** (278 mg, 0.295 mmol, 77 %) as dark-brown block crystals. Single crystals of **1'** suitable for X-ray diffraction studies were obtained by recrystallization from a hexane solution at −30 °C.

Characterization of 1': ^1H NMR (C_6D_{12} , rt): δ 2.90 (s, 18H, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 2.57 (s, 7H, $\mu\text{-H}$), 2.13 (s, 18H, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 0.88 (s, 27H, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 0.20 (s, 18H, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$). $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_{12} , rt): δ 131.1 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 124.7 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 113.1 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 28.5 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 21.0 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 18.6 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 14.0 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$), 0.2 (s, $\text{C}_5\text{Me}_4\text{Si}^t\text{BuMe}_2$). Anal. calcd. for $\text{C}_{45}\text{H}_{88}\text{Si}_3\text{Ti}_3\cdot\text{C}_6\text{H}_{14}$ (**1'**·hex): C, 64.94; H, 10.90. Found: C, 64.38; H, 10.40.

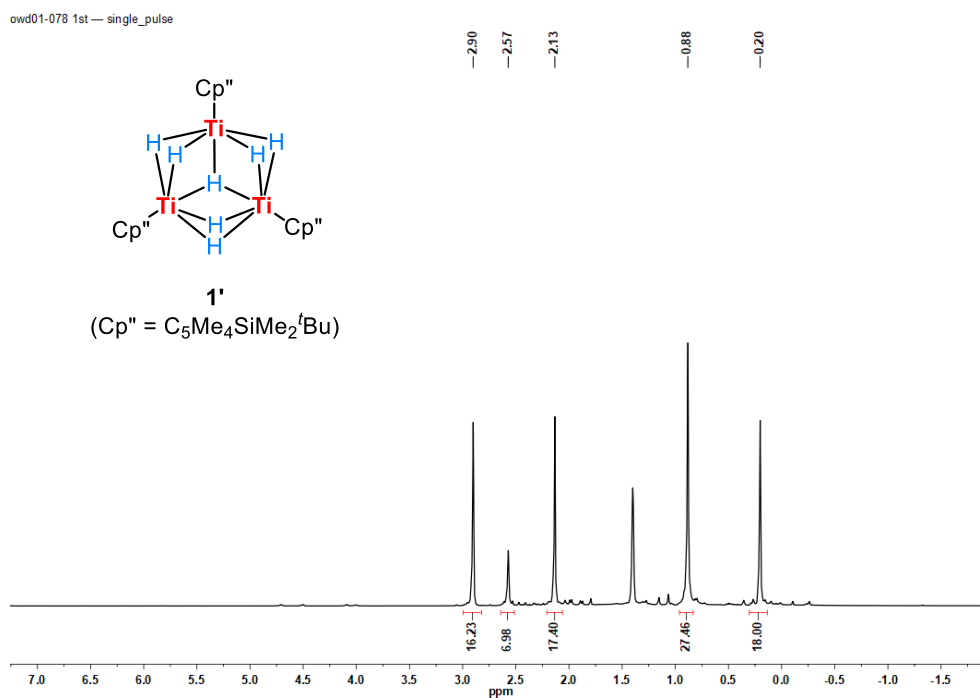


Figure S5. ^1H NMR spectrum of **1'** (C_6D_{12} , rt).

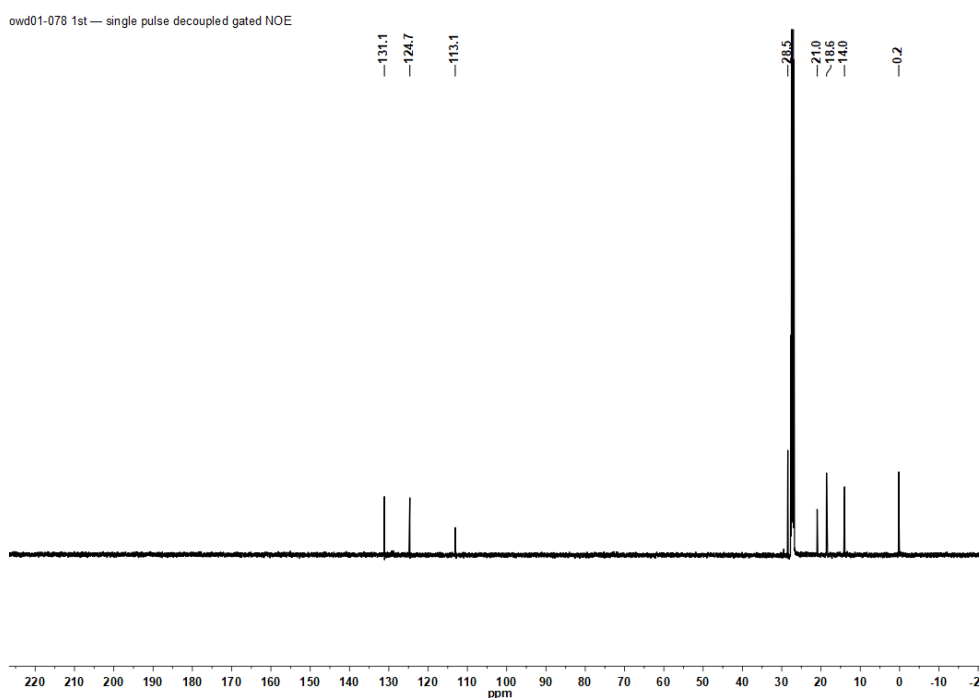
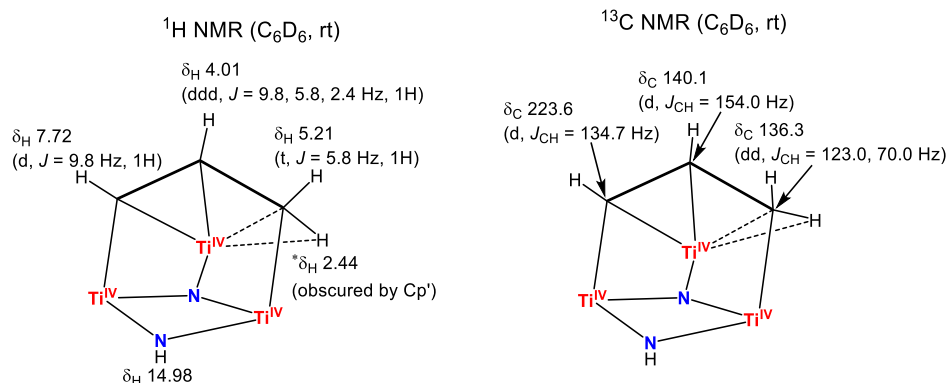


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1'** (C_6D_{12} , rt).

Reaction of 2 with propylene at 70 °C to yield 3: Propylene (1 atm) was introduced to a hexane solution (4 mL) of **2** (61.2 mg, 0.081 mmol) at room temperature. The mixture was heated at 70 °C and stirred for 2 days. After removal of the solvent under vacuum, the residual solid was recrystallized from dimethoxyethane (DME) at –30 °C to afford $[\{(C_5Me_4SiMe_3)Ti\}_3(\mu_3-\eta^2:\eta^1:\eta^1-CH-CH-CH_2-)(\mu_3-N)(\mu-NH)]$ (**3**) (38 mg, 0.048 mmol, 59%) as dark brown block crystals.

Heating 5 at 70 °C to yield 3: A benzene solution (0.5 mL) of **5** (14 mg, 0.018 mmol) in J. Young NMR tube was kept at 70 °C for 1 day. The color of the solution changed from dark purple to brown purple. After the reaction, the solution was evaporated and the residue was crystallized in DME at –30 °C to give **3** (12 mg, 0.015 mmol, 83%) as dark brown solid.

Characterization of 3: 1H NMR (C_6D_6 , rt): δ 14.98 (s, 1H, NH), 7.72 (d, J = 9.8 Hz, 1H, -CH-CH-CH₂-), 5.21 (t, J = 5.8 Hz, 1H, -CH-CH-CH₂-), 4.01 (ddd, J = 9.8, 5.8, 2.4 Hz, 1H, -CH-CH-CH₂-), 2.47 (s, 3H, $C_5Me_4SiMe_3$), 2.44 (-CH-CH-CH₂-, obscured by Cp'), 2.44 (s, 3H, $C_5Me_4SiMe_3$), 2.34 (s, 3H, $C_5Me_4SiMe_3$), 2.25 (s, 3H, $C_5Me_4SiMe_3$), 2.21 (s, 3H, $C_5Me_4SiMe_3$), 2.16 (s, 3H, $C_5Me_4SiMe_3$), 1.99 (s, 3H, $C_5Me_4SiMe_3$), 1.96 (s, 3H, $C_5Me_4SiMe_3$), 1.91 (s, 3H, $C_5Me_4SiMe_3$), 1.84 (s, 3H, $C_5Me_4SiMe_3$), 1.53 (s, 3H, $C_5Me_4SiMe_3$), 1.26 (s, 3H, $C_5Me_4SiMe_3$), 0.35 (s, 9H, $C_5Me_4SiMe_3$), 0.32 (s, 9H, $C_5Me_4SiMe_3$), 0.23 (s, 9H, $C_5Me_4SiMe_3$). $^{13}C\{^1H\}$ NMR (C_6D_6 , rt): δ 223.6 (s, -CH-CH-CH₂-), 140.1 (s, -CH-CH-CH₂-), 136.3 (s, -CH-CH-CH₂-), 128.6 (s, $C_5Me_4SiMe_3$), 128.5 (s, $C_5Me_4SiMe_3$), 127.7 (s, $C_5Me_4SiMe_3$), 126.0 (s, $C_5Me_4SiMe_3$), 124.8 (s, $C_5Me_4SiMe_3$), 124.1₇ (s, $C_5Me_4SiMe_3$), 124.1₅ (s, $C_5Me_4SiMe_3$), 123.8 (s, $C_5Me_4SiMe_3$), 123.4 (s, $C_5Me_4SiMe_3$), 123.3 (s, $C_5Me_4SiMe_3$), 122.1 (s, $C_5Me_4SiMe_3$), 120.9 (s, $C_5Me_4SiMe_3$), 116.3 (s, $C_5Me_4SiMe_3$), 115.5 (s, $C_5Me_4SiMe_3$), 112.9 (s, $C_5Me_4SiMe_3$), 16.0 (s, $C_5Me_4SiMe_3$), 15.4₉ (s, $C_5Me_4SiMe_3$), 15.4₆ (s, $C_5Me_4SiMe_3$), 15.0 (s, $C_5Me_4SiMe_3$), 12.5 (s, $C_5Me_4SiMe_3$), 12.3 (s, $C_5Me_4SiMe_3$), 12.1 (s, $C_5Me_4SiMe_3$), 12.0 (s, $C_5Me_4SiMe_3$), 11.8 (s, $C_5Me_4SiMe_3$), 11.2 (s, $C_5Me_4SiMe_3$), 2.6₂ (s, $C_5Me_4SiMe_3$), 2.5₆ (s, $C_5Me_4SiMe_3$). ^{13}C NMR (C_6D_6 , non-decoupling, rt): δ 223.6 (d, J_{CH} = 134.7 Hz, -CH-CH-CH₂-), 140.1 (d, J_{CH} = 154.0 Hz, -CH-CH-CH₂-), 136.3 (dd, J_{CH} = 123.0, 70.0 Hz, -CH-CH-CH₂-). 1H - 1H COSY (C_6D_6 , rt): δ_H 7.72-4.01; δ_H 5.21-4.01, 2.48; δ_H 4.01-7.72, 5.21. 1H - ^{13}C HMQC (C_6D_6 , rt): δ_H 7.72- δ_C 223.6; δ_H 4.01- δ_C 140.1; δ_H 5.21, 2.48- δ_C 136.3. IR (KBr, Nujol mulls, cm⁻¹): 3372 (ν_{NH} , m), 2952 (vs), 2919 (vs), 2854 (vs), 1454 (s), 1377 (s), 1329 (s), 1247 (s), 1211 (w), 1130 (m), 1024 (s), 833 (vs), 754 (s), 693 (s), 665 (s), 633 (s), 551 (s). Anal. calcd. for $C_{39}H_{68}N_2Si_3Ti_3$: C, 59.08; H, 8.64; N, 3.53. Found: C, 58.49; H, 8.74; N, 3.33.



Formation and characterization of ^{15}N -labelled **3- ^{15}N :** The ^{15}N -enriched compound $[\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-}\eta^2\text{:}\eta^1\text{:}\eta^1\text{-CH-CH-CH}_2\text{-})(\mu_3\text{-}^{15}\text{N})(\mu\text{-}^{15}\text{NH})]$ (**3**- ^{15}N) was obtained from the reaction of $[\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-}^{15}\text{N})(\mu\text{-}^{15}\text{NH})(\mu\text{-H})_2]$ (**2**- ^{15}N) (6 mg, 0.008 mmol) with propylene (1 atm) in C_6D_6 (0.4 mL) at 70 °C for 16 h. ^1H NMR (C_6D_6 , rt): δ 14.98 (d, $J_{\text{NH}} = 66.0$ Hz, $^{15}\text{N}\text{-H}$). $^{15}\text{N}\{^1\text{H}\}$ NMR (C_6D_6 , rt): δ 499.4 (s, $\mu_3\text{-}^{15}\text{N}$), 97.6 (s, $\mu\text{-}^{15}\text{NH}$). IR (KBr, Nujol mulls, cm^{-1}): 3365 ($\nu^{15}\text{NH}$, m), 2951 (vs), 2913 (vs), 2853 (vs), 1454 (s), 1379 (s), 1328 (s), 1248 (s), 1212 (w), 1131 (m), 1022 (s), 833 (vs), 754 (s), 695 (s), 652 (s), 634 (s), 541 (s).

The signals of the propenyl unit ($\text{-CH-CH-CH}_2\text{-}$) in **3** were observed at δ_{H} 7.72 (d, $J = 9.8$ Hz), 5.21 (t, $J = 5.8$ Hz), 4.01 (ddd, $J = 9.8, 5.8, 2.4$ Hz), and 2.44 (overlapped with Cp' methyl signals) in the ^1H NMR spectrum, and δ_{C} 223.6 (d, $J_{\text{CH}} = 134.7$ Hz), 140.1 (d, $J_{\text{CH}} = 154.0$ Hz), and 136.3 (dd, $J_{\text{CH}} = 123.0, 70.0$ Hz) in the ^{13}C NMR spectrum (^1H non-decoupling). Further studies by two-dimensional correlation spectroscopy (2D COSY) and heteronuclear multiple quantum coherence (HMQC) NMR supported the formation of propenyl unit. In addition, the ^{13}C signal at δ_{C} 136.3 showed relatively small $^{13}\text{C}\text{-}^1\text{H}$ coupling constant ($J_{\text{CH}} = 70.0$ Hz), suggesting the presence of an agostic $\text{C-H}\cdots\text{Ti}$ interaction⁵. The $^{15}\text{N}\text{-H}$ proton in **3**- ^{15}N was observed at δ_{H} 14.98 ($J_{\text{NH}} = 66.0$ Hz) in the ^1H NMR spectrum. In the infrared spectroscopy (IR) spectrum (KBr, Nujol mulls), the $^{14}\text{N}\text{-H}/^{15}\text{N}\text{-H}$ stretching vibrations in **3/3**- ^{15}N were observed at ν 3372/3365 cm^{-1} .

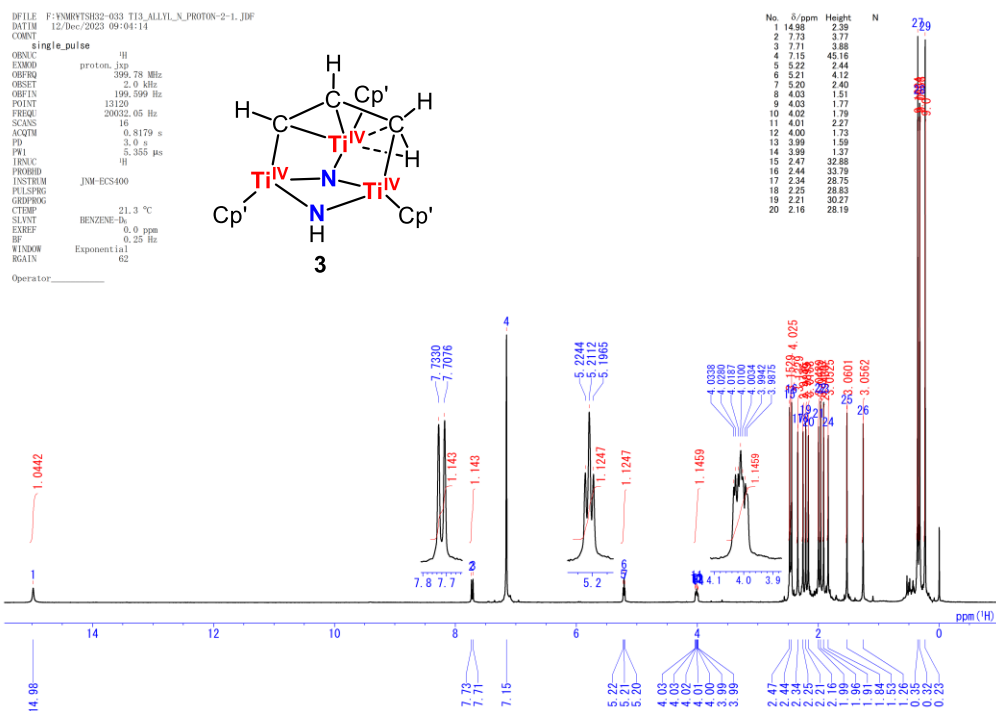


Figure S7. ^1H NMR spectrum of **3** (C_6D_6 , rt). No significant changes in the resonance signals of the $\text{C}_5\text{Me}_4\text{SiMe}_3$ ligands were observed in the VT- ^1H NMR experiment ($-90\text{ }^\circ\text{C} \sim 80\text{ }^\circ\text{C}$).

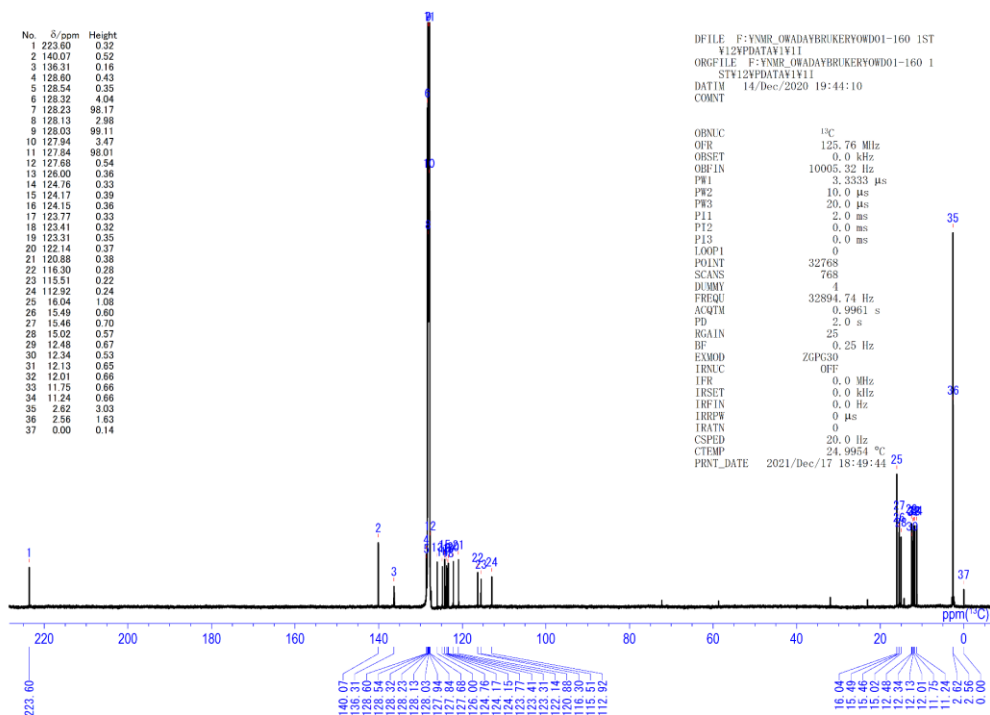


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **3** (C_6D_6 , rt).

No.	δ /ppm	Height
1	224.21	0.08
2	224.15	0.10
3	223.09	0.10
4	141.49	0.08
5	140.68	0.16
6	140.64	0.12
7	139.45	0.15
8	137.07	0.04
9	136.98	0.04
10	136.52	0.03
11	136.41	0.04
12	136.08	0.04
13	135.99	0.03
14	135.52	0.03
15	135.44	0.03

DFILE F:\NMR\TSH29\TSH29-144 T13_C3_N TOTAL 13C_NON
 -DECOUPLING, ALS
 DATIM 26/May/2021 19:45:09
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 OBNUC ^{13}C
 EXM00 ZG6D30
 OBFRQ 125.76 MHz
 OBSET 0.0 kHz
 OBF1N 10901.65 Hz
 POINT 32768
 FREQU 37878.79 Hz
 SCANS 1026
 ACQTM 0.8651 s
 PD 2.0 s
 PW1 3.3333 μs
 IRNLC OFF
 PROBD Z125995_0002 (CP DCH 500S1 C/H-D
 INSTRUM SPECT
 PULSPRG ZG6D30
 GRDPRG
 CTMP 26.8058 $^{\circ}\text{C}$
 SLVT C4s
 EXREF 280.9425 ppm
 BF 0.578 Hz
 WINDOW Exponential
 RGAIN 25
 Operator_____

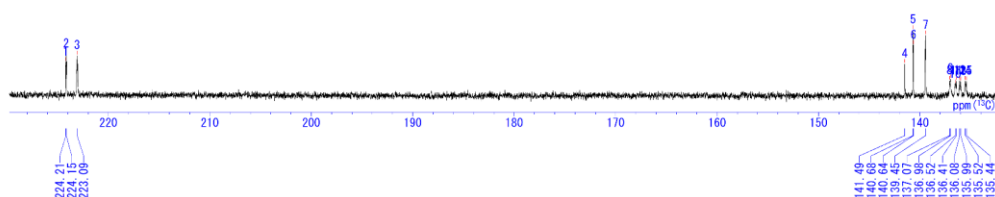


Figure S9. $^{13}\text{C}\{^1\text{H non decoupling}\}$ NMR spectrum of **3** (C_6D_6 , rt).

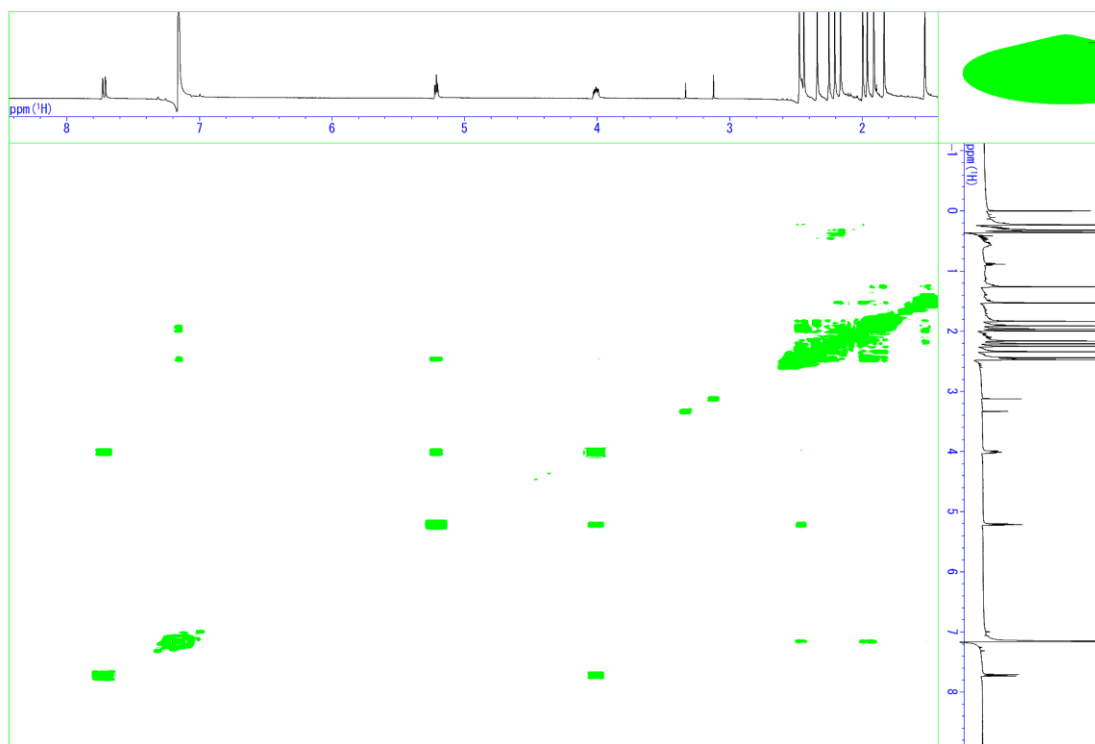


Figure S10. $^1\text{H}-^1\text{H}$ COSY spectrum of **3** (C_6D_6 , rt).

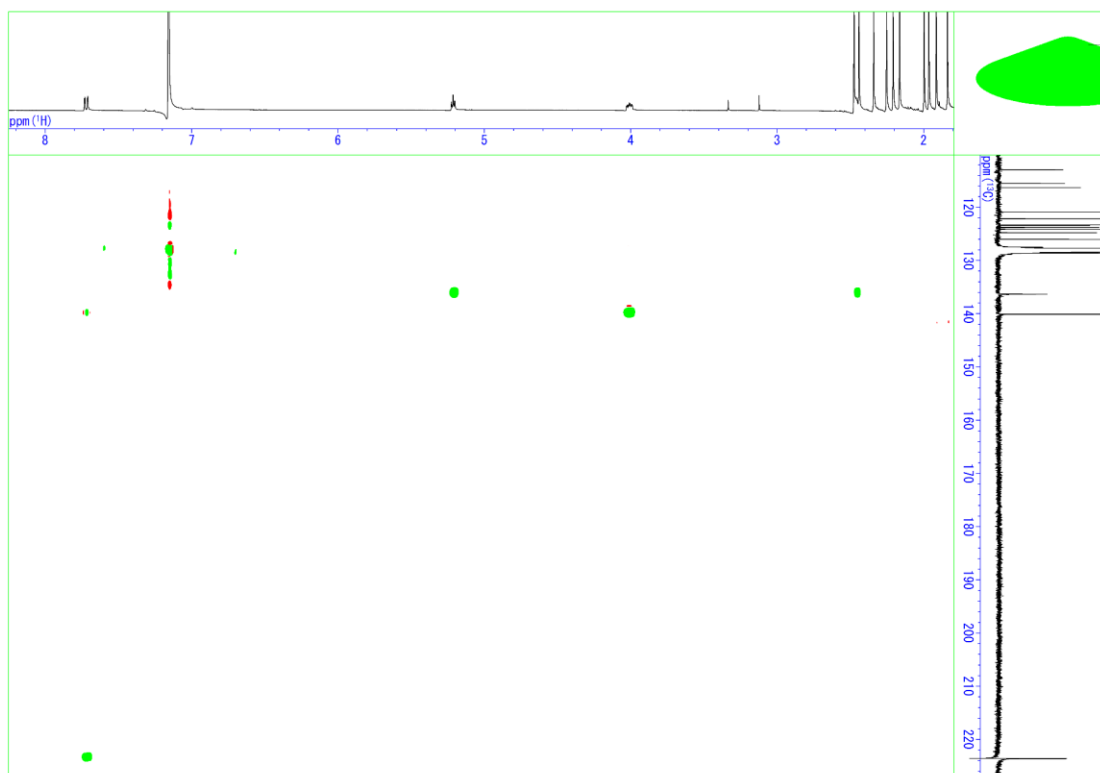


Figure S11. ^{13}C - ^1H HMQC spectrum of **3** (C_6D_6 , rt).

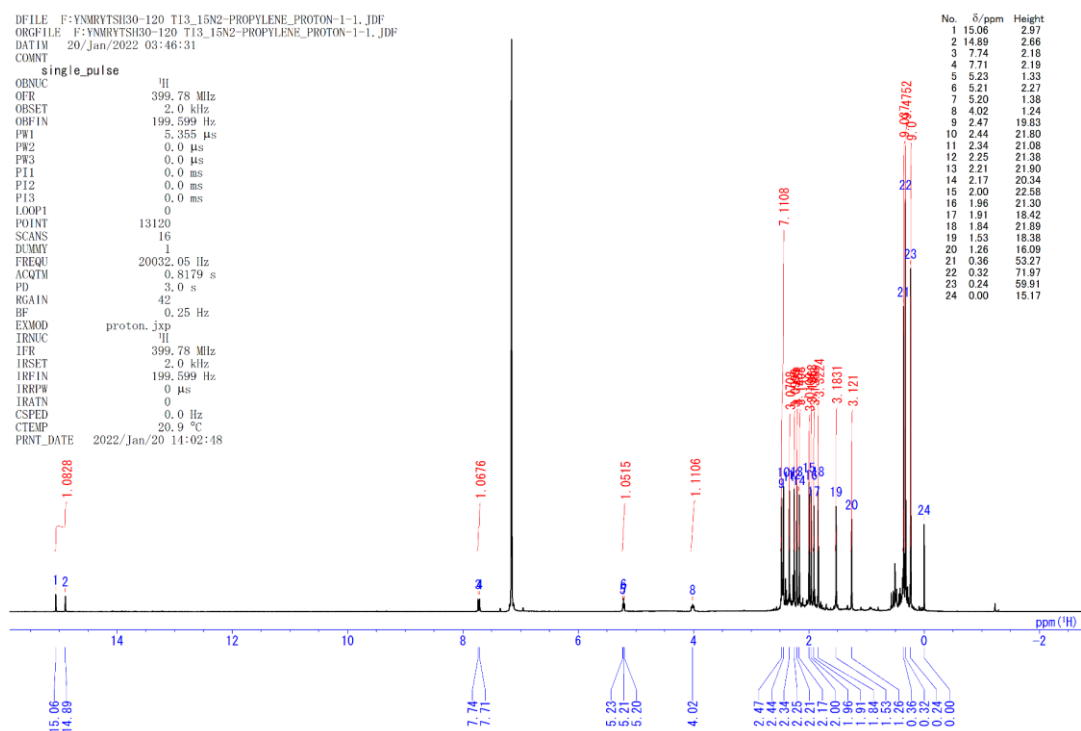


Figure S12. ^1H NMR spectrum of **3**- ^{15}N (C_6D_6 , rt).

DFILE F:\NMR\TSH30-120 TI3_15N2-PROPYLENE_NITROGEN-1-1.JDF
 ORGFILE F:\NMR\TSH30-120 TI3_15N2-PROPYLENE_NITROGEN-1-1.JD
 F
 DATIM 20/Jan/2022 05:05:12
 COMNT single pulse decoupled gated NOE
 OBNUC ^{15}N
 OFR 40.52 MHz
 ORSET 5.0 kHz
 OFFIN -88.2179 Hz
 PW1 5.0367 μs
 PW2 0.0 μs
 PW3 0.0 μs
 PT1 0.0 ms
 PT2 0.0 ms
 PT3 0.0 ms
 LOOP1 0
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 SCANS 1741
 DUMMY 4
 FREQU 40584.41 Hz
 ACQTM 0.8074 s
 PD 1.0 s
 RGAIN 50
 BF 0.25 Hz
 EXMOD carbon.jxp
 IERUC ^1H
 IFR 399.78 MHz
 IRSET 2.0 kHz
 IRRFIN 199.599 Hz
 IRRPW 115 μs
 IRATN 0
 CSPED 0.0 Hz
 CTEMP 21.0 $^{\circ}\text{C}$
 PRINT_DATE 2022/Jan/20 14:09:23

No.	δ/ppm	Height
1	499.36	22.90
2	97.63	46.66

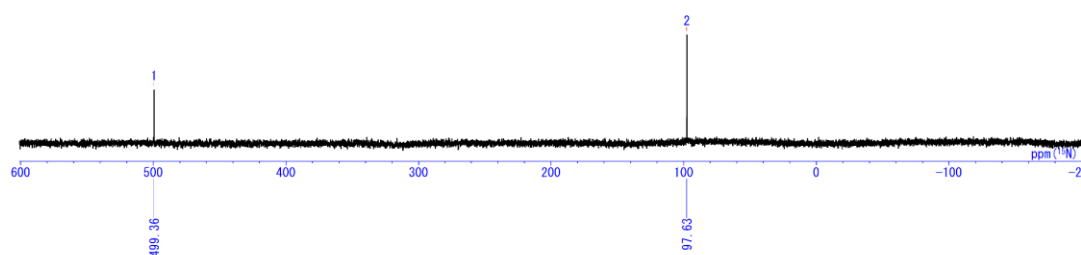


Figure S13. $^{15}\text{N}\{^1\text{H}\}$ NMR spectrum of $3\text{-}^{15}\text{N}$ (C_6D_6 , rt).

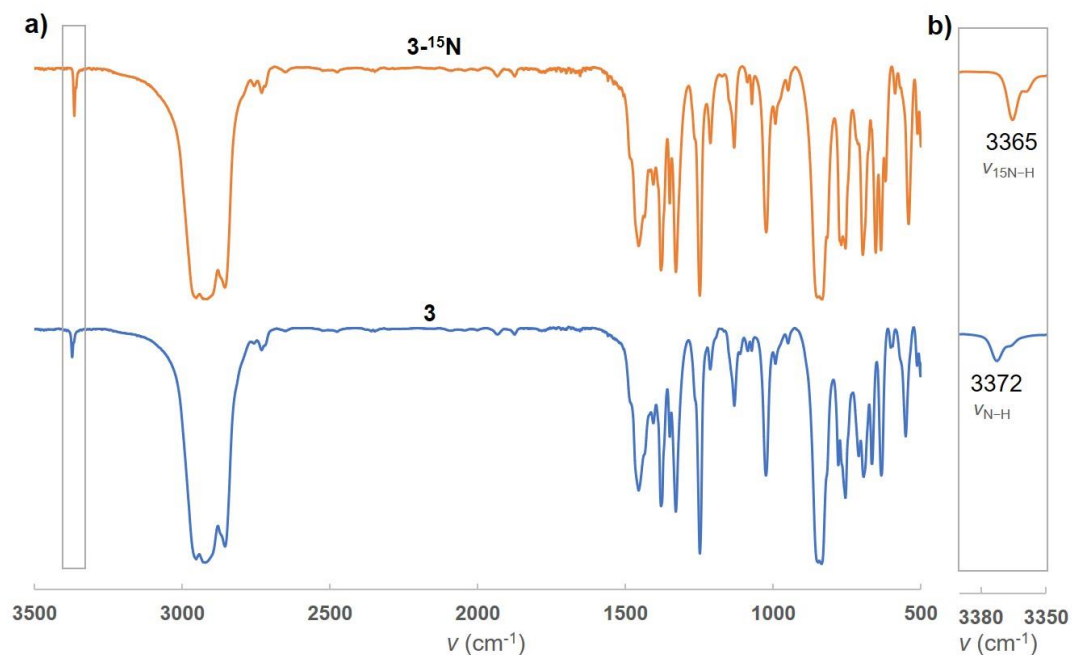
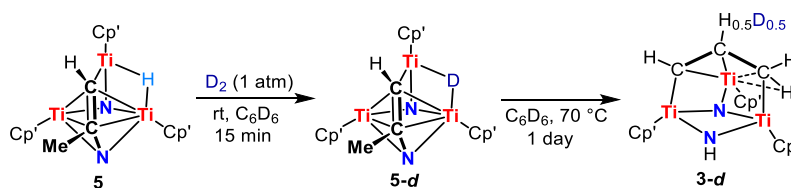


Figure S14. IR spectra of isotopologues of **3**. **a)** Stacked IR spectra of **3** and $3\text{-}^{15}\text{N}$. **b)** Stacked partial IR spectra of **3** and $3\text{-}^{15}\text{N}$.

Heating deuterium-labelled 5-*d* at 70 °C to yield deuterium-labelled 3-*d*:



A J. Young valve NMR sample tube was charged with 0.4 mL of C_6D_6 and complex **5** (5 mg). The solution was frozen in liquid nitrogen, degassed and 1 atm of D_2 gas was added. The solution was kept at room temperature for 15 min and the 1H NMR monitoring showed quantitative formation of the deuterated complex $[{(C_5Me_4SiMe_3)Ti}_3(\mu_3-\eta^3:\eta^3:\eta^1-CH-C(CH_3)N-)(\mu_3-N)(\mu-D)]$ (**5-d**). After the confirmation of the deuteration, D_2 gas was removed from the tube and the solution of **5-d** was kept at 70 °C. After 1 day, the partially deuterated complex $[{(C_5Me_4SiMe_3)Ti}_3(\mu_3-\eta^3:\eta^1:\eta^1-CH-CH_{0.5}D_{0.5}-CH_2-)(\mu_3-N)(\mu-NH)]$ (**3-d**) was obtained quantitatively by the 1H NMR.

Characterization of 3-d: 1H NMR (C_6D_6 , rt): δ 14.97 (s, 1H, NH), 7.72 (d, $J = 6.1$ Hz, 1H, $-CH-CH_{0.5}D_{0.5}-CH_2-$), 5.21 (d, $J = 4.8$ Hz, 1H, $-CH-CH_{0.5}D_{0.5}-CH_2-$), 4.01 (m, 0.5H, $-CH-CH_{0.5}D_{0.5}-CH_2-$). 2H NMR (C_6H_6 , rt): δ 4.1 (s, $-CH-CH_{0.5}D_{0.5}-CH_2-$).

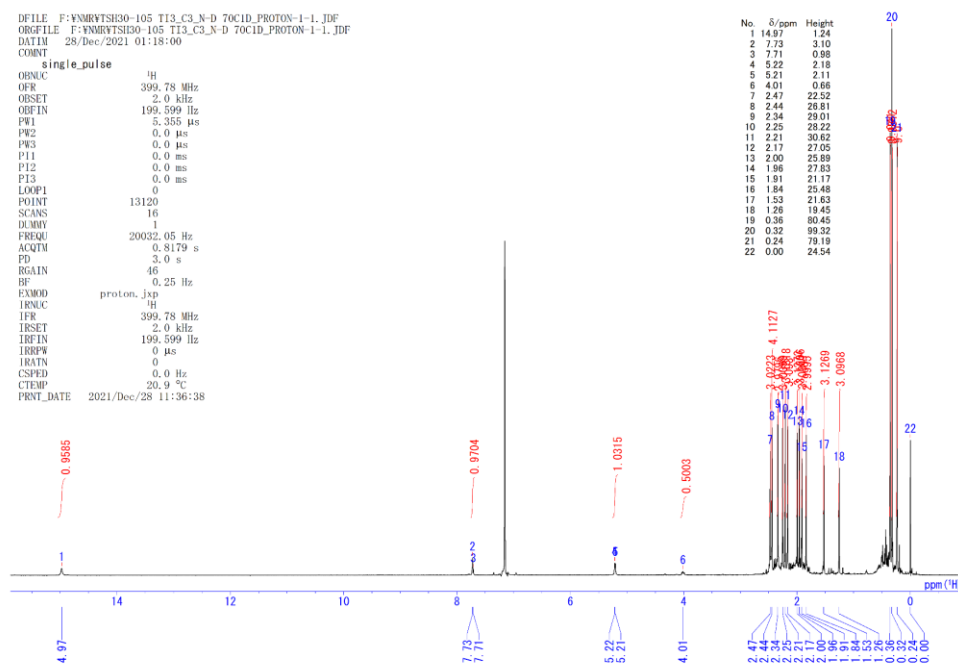


Figure S15. 1H NMR spectrum of **3-d** (C_6D_6 , rt).

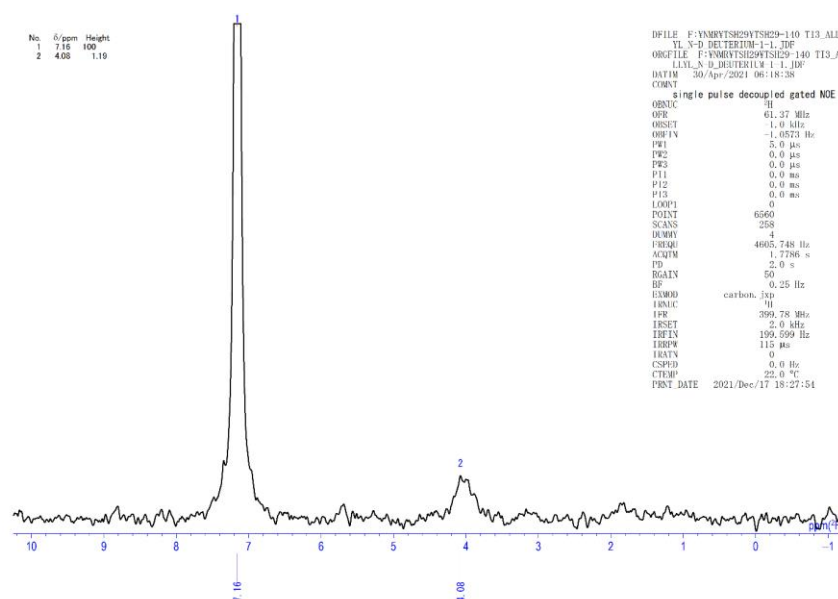


Figure S16. ^2H NMR spectrum of **3-d** (C_6H_6 , rt).

Reaction of 1 with propylene to yield 4a: A hexane solution (3.0 mL) of **1** (75 mg, 0.10 mmol) in 50 mL Schlenk tube equipped with a J. Young valve was frozen in liquid nitrogen, pumped, and backfilled with atmospheric pressure of propylene. The solution was stirred at room temperature for 1 h. The solution turned from brown to dark red-brown. After removal of the solvent under vacuum, the resulting solid was dissolved in DME, concentrated and crystallized at $-30\text{ }^\circ\text{C}$ to give dark brown crystals of $[\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-}\eta^2\text{:}\eta^2\text{:}\eta^1\text{-C=CCH}_3)(\mu\text{-H})_3(\mu_3\text{-H})]$ (**4a**) (65 mg, 0.085 mmol, 85%). Single crystals of **4a** suitable for X-ray diffraction studies were obtained by recrystallization from a hexane solution at $-30\text{ }^\circ\text{C}$.

Characterization of 4a: ^1H NMR (C_6D_6 , rt): δ 6.43 (q, $J_{\text{HH}} = 14.5\text{ Hz}$, 1H, $\mu_3\text{-H}$), 2.29 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 1.90 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 1.74 (s, 3H, -C=CCH_3), 0.38 (s, 27H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), -2.30 (d, $J_{\text{HH}} = 14.5\text{ Hz}$, 3H, $\mu\text{-H}$). $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , rt): δ 338.3 (s, -C=CCH_3), 247.0 (s, -C=CCH_3), 128.7 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 124.5 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 116.2 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 23.3 (s, -C=CCH_3), 16.5 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 12.4 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 2.9 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$). IR (KBr, Nujol mulls, cm^{-1}): 2952 (vs), 2916 (vs), 2954 (vs), 1456 (s), 1379 (s), 1331 (s), 1240 (s), 1127 (m), 1085 (w), 1025 (s), 935 (w), 835 (vs), 735 (s), 684 (s), 632 (s). Anal. calcd. for $\text{C}_{39}\text{H}_{70}\text{Si}_3\text{Ti}_3$: C, 61.08; H, 9.20. Found: C, 60.37; H, 9.17.

The ^1H NMR spectrum of **4a** showed quartet and doublet signals at δ_{H} 6.43 (q, $J_{\text{HH}} = 14.5\text{ Hz}$, 1H) and -2.30 (d, $J_{\text{HH}} = 14.5\text{ Hz}$, 3H), which could be assigned to the $\mu_3\text{-}$ and $\mu\text{-}$ bridging hydride ligands. The signal at δ_{H} 1.74 (3H) could be assigned to the methyl group in the propenylidene unit. Only one set of resonance signals of the Cp' ligands was observed at δ_{H} 2.29 (18H), 1.90 (18H), and 0.38 (27H) at room temperature (Fig. S17), demonstrating that the structure of **4a** is highly fluxional (Fig. S21). In the $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4a**, the coordinated propenylidene carbons were appeared at δ_{C} 338.3 ($\mu_3\text{-C}$), 247.0 ($\mu\text{-C}$), and 23.3 (Me) (Fig. S18).

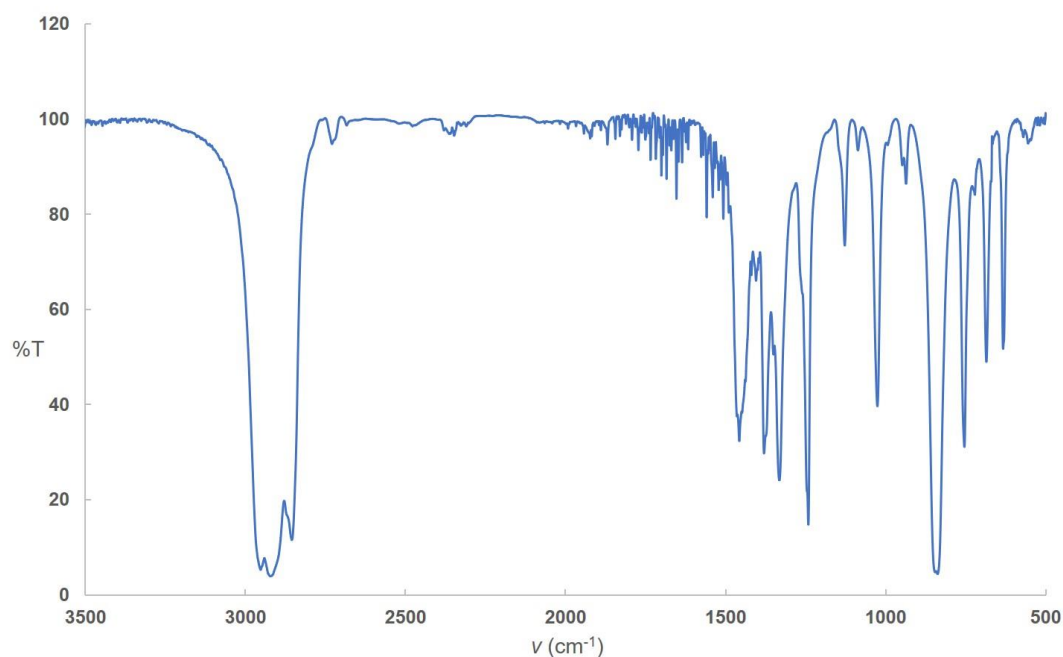


Figure S19. IR spectrum of **4a**.

^1H NMR monitoring the reaction of **1 with propylene:** A J. Young valve NMR sample tube was charged with 0.4 mL of $\text{THF-}d_8$ and complex **1** (4 mg). The solution was frozen in liquid nitrogen, degassed and 1 atm of propylene gas was added. The reaction was monitored by ^1H NMR at -20°C to room temperature. An intermediate species was observed during the reaction. After 1 h at room temperature, the intermediate species disappeared and complex **4a** was formed quantitatively.

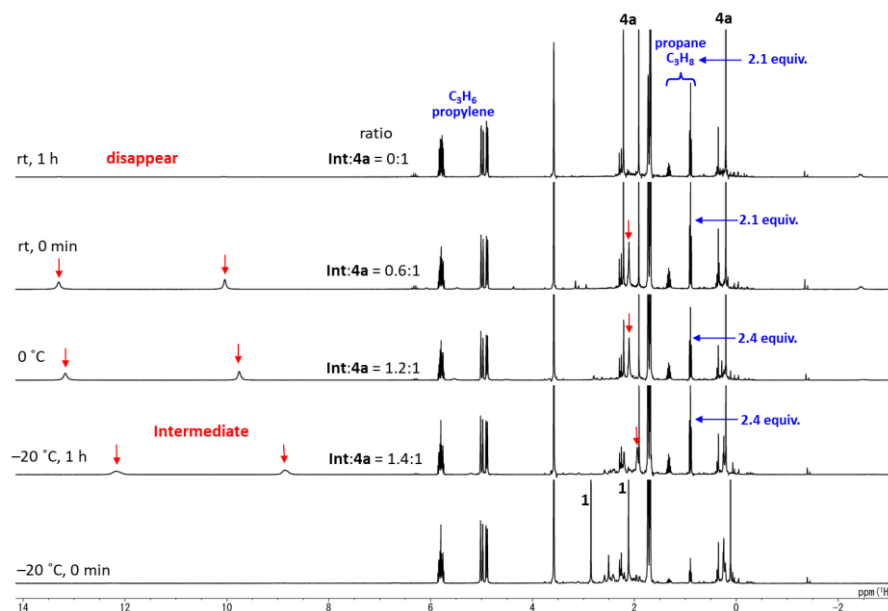


Figure S20. ^1H NMR monitoring the reaction of **1** with propylene (1 atm) ($\text{THF-}d_8$, -20°C ~rt).

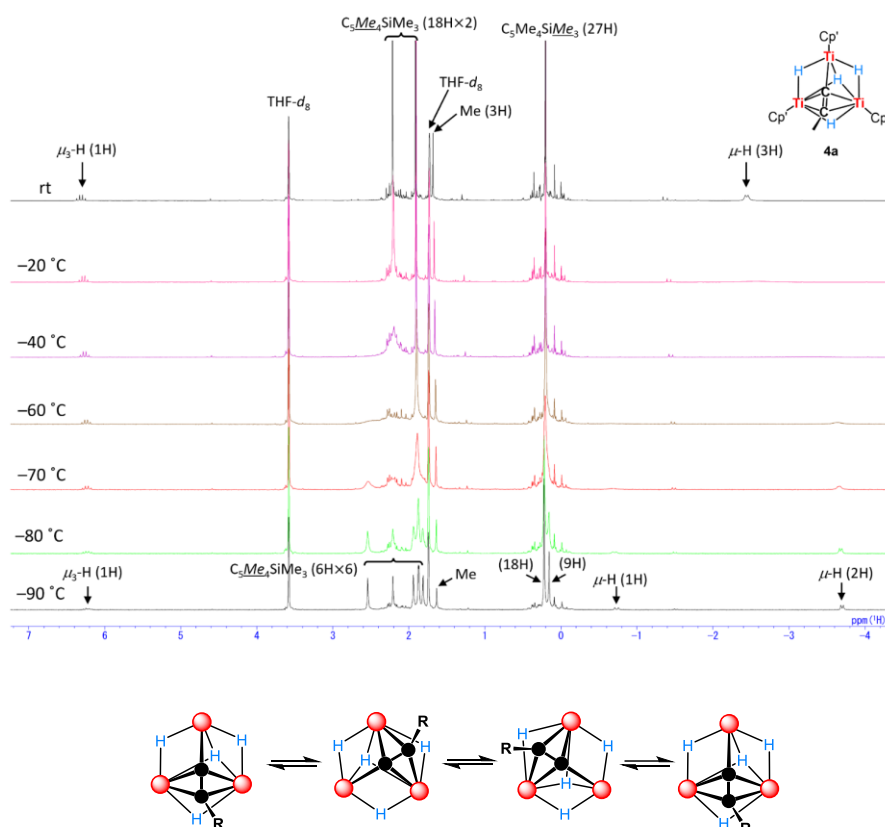


Figure S21. VT- ^1H NMR spectra of **4a** (THF- d_8) (top), and plausible dynamic process (bottom). At $-90\text{ }^\circ\text{C}$, the trimethylsilyl group of Cp' and $\mu\text{-H}$ ligands were separated in a 2:1 ratio, which is consistent with the structure shown in Fig. 1. The results demonstrate the existence of a quick site-change process of the $\mu\text{-carbon}$ unit among the three Ti-Ti edges.

Reaction of 1 with 1-butene to yield 4b: A hexane solution (4.0 mL) of **1** (115 mg, 0.157 mmol) in 50 mL Schlenk tube equipped with a J. Young valve was frozen in liquid nitrogen, pumped, and backfilled with atmospheric pressure of 1-butene. The solution was stirred at room temperature for 1 h. The solution turned from brown to dark red-brown. After removal of the solvent under vacuum, the resulting solid was dissolved in pentane (1st batch) / DME (2nd batch), concentrated and crystallized at $-30\text{ }^\circ\text{C}$ to give dark brown crystals of $[\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-}\eta^2\text{:}\eta^2\text{:}\eta^1\text{-C=CC}_2\text{H}_5)(\mu\text{-H})_3(\mu_3\text{-H})]$ (**4b**) (81 mg, 0.104 mmol, 66%).

Characterization of 4b: ^1H NMR (C_6D_6 , rt): δ 5.91 (q, $J = 14.7\text{ Hz}$, 1H, $\mu_3\text{-H}$), 2.30 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 2.25 (q, $J = 7.3\text{ Hz}$, 2H, $\mu_3\text{-C=CC}_2\text{H}_5$), 1.93 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 0.63 (t, $J = 7.3\text{ Hz}$, 3H, $\mu_3\text{-C=CC}_2\text{H}_5$), 0.38 (s, 27H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), -2.32 (d, $J = 14.7\text{ Hz}$, 3H, $\mu\text{-H}$). $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , rt): δ 338.8 (s, $\mu_3\text{-C=CC}_2\text{H}_5$), 255.9 (s, $\mu_3\text{-C=CC}_2\text{H}_5$), 128.9 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 124.5 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 116.4 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 32.0 (s, $\mu_3\text{-C=CC}_2\text{H}_5$), 16.6 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 16.4 (s, $\mu_3\text{-C=CC}_2\text{H}_5$), 12.4 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 2.9 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$). Anal. calcd. for $\text{C}_{40}\text{H}_{72}\text{Si}_3\text{Ti}_3$: C, 61.53; H, 9.29. Found: C, 61.60; H, 9.22.

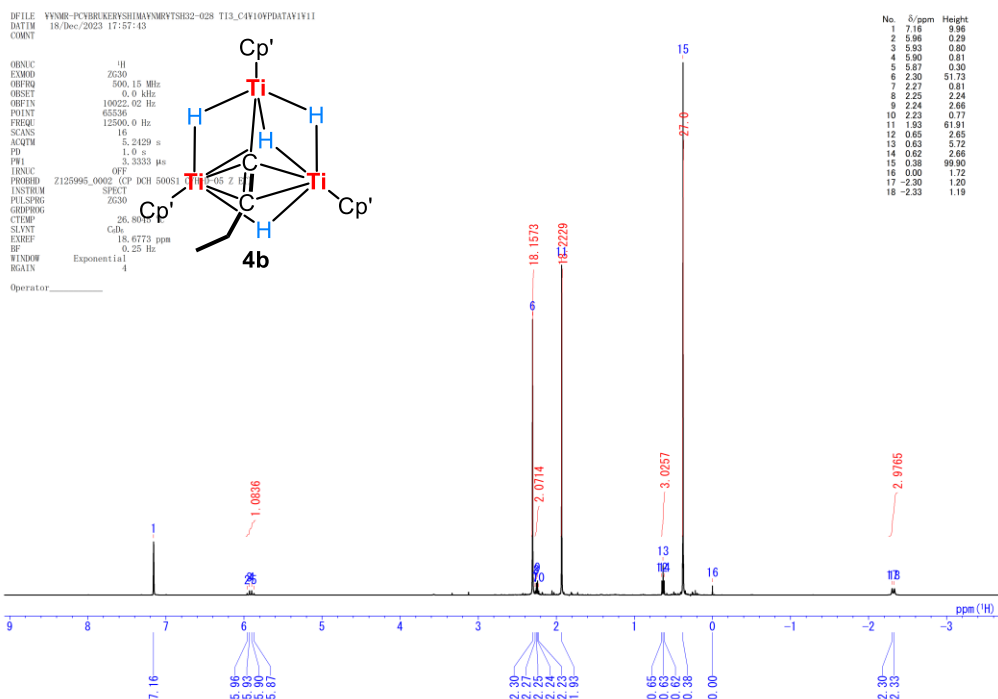


Figure S22. ^1H NMR spectrum of **4b** (C_6D_6 , rt).

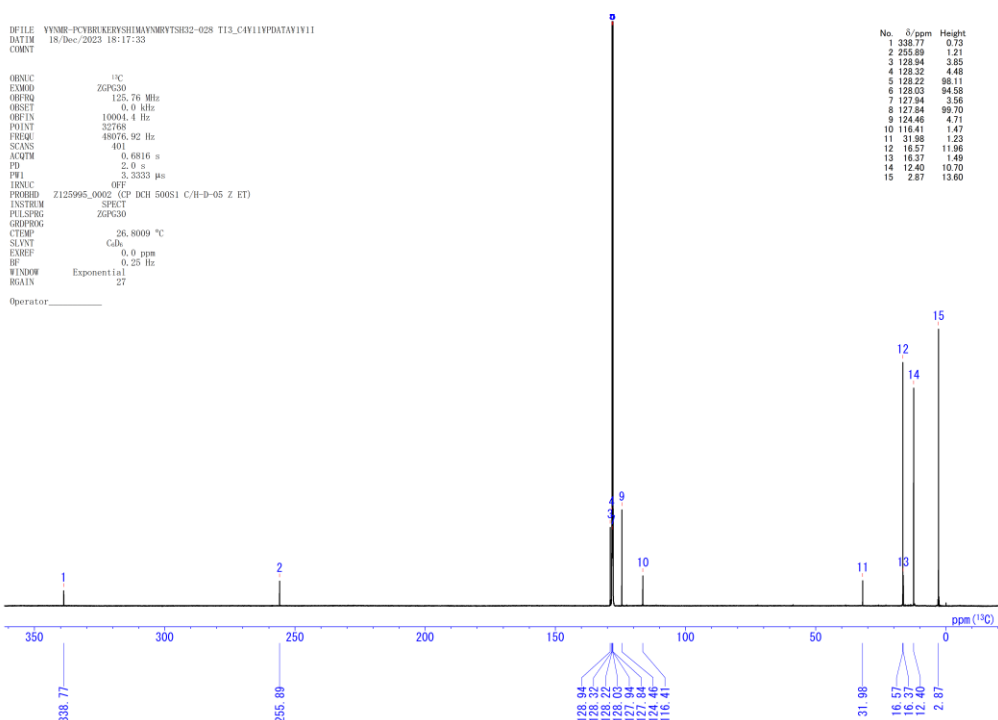
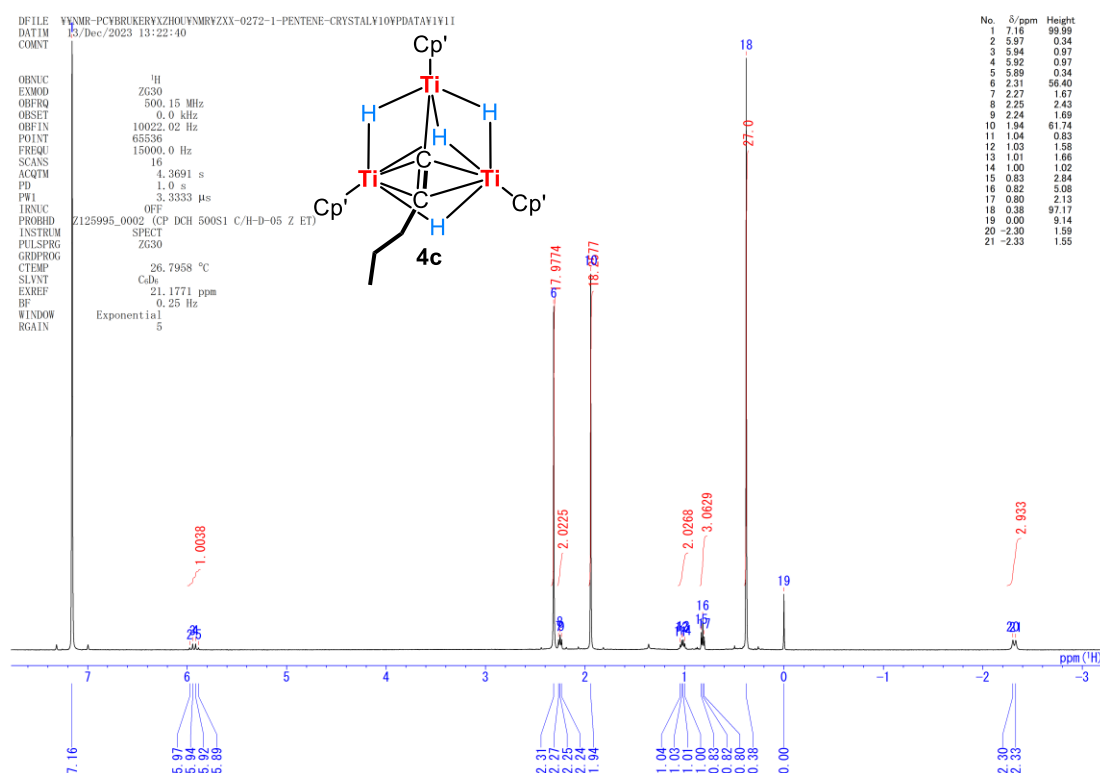


Figure S23. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4b** (C_6D_6 , rt).

Reaction of 1 with 1-pentene to yield 4c: To a 2.0 mL hexane solution of **1** (90 mg, 0.12 mmol) was added 1-pentene (80 μL , 0.73 mmol) in a 50-mL round-bottomed flask in an Ar glovebox. The solution was kept at room temperature for 1 h. The solution turned from brown to dark red-brown. After removal of the solvent under vacuum, the resulting solid was dissolved in pentane and crystallized at $-30\text{ }^\circ\text{C}$ to give dark brown

crystals of $[(C_5Me_4SiMe_3)Ti]_3(\mu_3-\eta^2:\eta^1-C=CCH_2CH_2CH_3)(\mu-H)_3(\mu_3-H)]$ (**4c**) (72 mg, 0.091 mmol, 74%).

Characterization of 4c: 1H NMR (C_6D_6 , rt): δ 5.93 (q, $J = 14.5$ Hz, 1H, μ_3-H), 2.31 (s, 18H, $C_5Me_4SiMe_3$), 2.25 (t, $J = 7.5$ Hz, 2H, $\mu_3-C=CC_3H_7$), 1.94 (s, 18H, $C_5Me_4SiMe_3$), 1.02 (sext, $J = 7.5$ Hz, 2H, $\mu_3-C=CC_3H_7$), 0.82 (t, $J = 7.5$ Hz, 3H, $\mu_3-C=CC_3H_7$), 0.38 (s, 27H, $C_5Me_4SiMe_3$), -2.32 (d, $J = 14.5$ Hz, 3H, $\mu-H$). $^{13}C\{^1H\}$ NMR (C_6D_6 , rt): δ 338.2 (s, $\mu_3-C=CC_3H_7$), 253.8 (s, $\mu_3-C=CC_3H_7$), 129.0 (s, $C_5Me_4SiMe_3$), 124.5 (s, $C_5Me_4SiMe_3$), 116.5 (s, $C_5Me_4SiMe_3$), 41.4 (s, $\mu_3-C=CC_3H_7$), 25.1 (s, $\mu_3-C=CC_3H_7$), 16.6 (s, $C_5Me_4SiMe_3$), 14.3 (s, $\mu_3-C=CC_3H_7$), 12.5 (s, $C_5Me_4SiMe_3$), 2.9 (s, $C_5Me_4SiMe_3$). Anal. calcd. for $C_{41}H_{74}Si_3Ti_3 \cdot (C_5H_{12})_{0.5}$: C, 62.88; H, 9.70. Found: C, 63.29; H, 9.39.



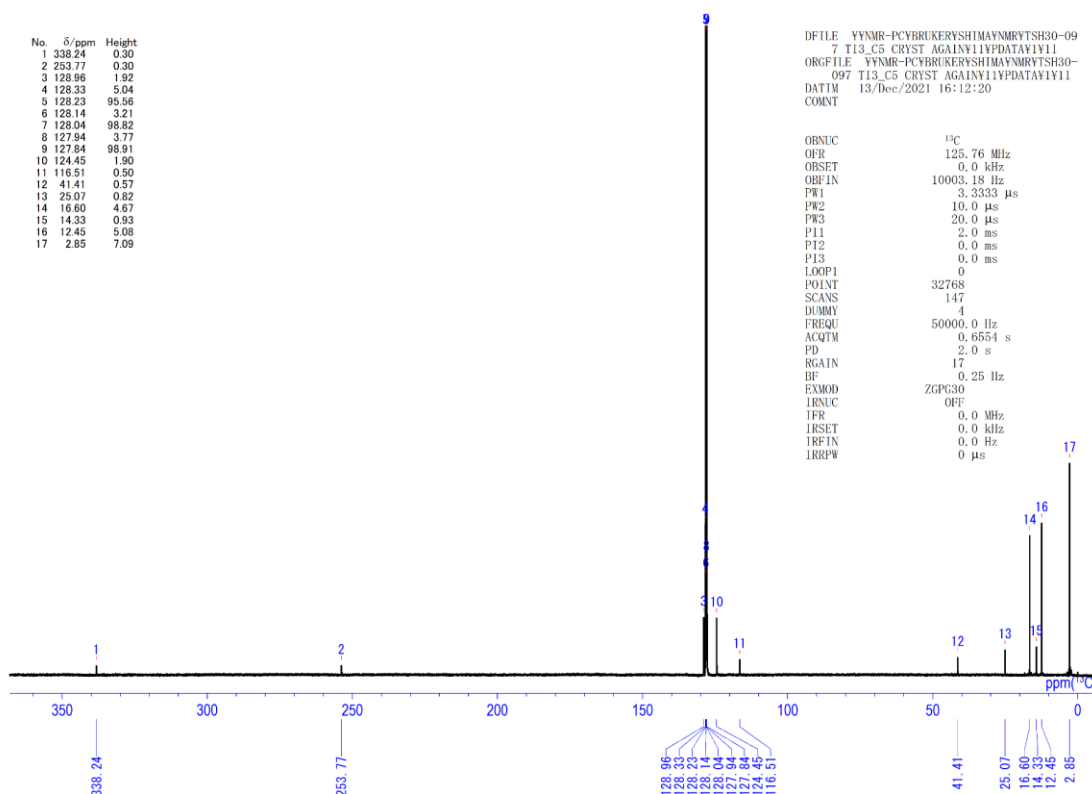


Figure S25. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4c** (C_6D_6 , rt).

Reaction of **1 with 1-hexene to yield **4d**:** To a 2.0 mL hexane solution of **1** (100 mg, 0.137 mmol) was added 1-hexene (100 μL , 0.8 mmol) in a 50-mL round-bottomed flask in an Ar glovebox. The solution was kept at room temperature for 2 h. The solution turned from brown to dark red-brown. After removal of the solvent under vacuum, the resulting solid was dissolved in pentane (1st batch), DME (2nd batch) and crystallized at $-30\text{ }^\circ\text{C}$ to give dark brown crystals of $[\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-}\eta^2\text{:}\eta^2\text{:}\eta^1\text{-C=CCH}_2\text{CH}_2\text{CH}_2\text{CH}_3)(\mu\text{-H})_3(\mu_3\text{-H})]$ (**4d**) (81 mg, 0.10 mmol, 73%).

The reaction of **1** with an α,ω -diene such as 1,5-hexadiene gave **4d** (~60% yield), similar to the reaction of **1** with 1-hexene.

Characterization of **4d:** ^1H NMR (C_6D_6 , rt): δ 5.92 (q, $J = 14.5\text{ Hz}$, 1H, $\mu_3\text{-H}$), 2.31 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 2.28 (m, 2H, $\mu_3\text{-C=CC}_4\text{H}_9$), 1.95 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 1.21 (sext, $J = 7.4\text{ Hz}$, 2H, $\mu_3\text{-C=CC}_4\text{H}_9$), 1.00 (quint, $J = 7.5\text{ Hz}$, 2H, $\mu_3\text{-C=CC}_4\text{H}_9$), 0.89 (t, $J = 7.5\text{ Hz}$, 3H, $\mu_3\text{-C=CC}_4\text{H}_9$), 0.38 (s, 27H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), -2.33 (d, $J = 14.5\text{ Hz}$, 3H, $\mu\text{-H}$). $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , rt): δ 338.2 (s, $\mu_3\text{-C=CC}_4\text{H}_9$), 254.0 (s, $\mu_3\text{-C=CC}_4\text{H}_9$), 129.0 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 124.4 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 116.5 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 38.9 (s, $\mu_3\text{-C=CC}_4\text{H}_9$), 34.1 (s, $\mu_3\text{-C=CC}_4\text{H}_9$), 23.0 (s, $\mu_3\text{-C=CC}_4\text{H}_9$), 16.6 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 14.4 (s, $\mu_3\text{-C=CC}_4\text{H}_9$), 12.4 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 2.9 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$). Anal. calcd. for $\text{C}_{42}\text{H}_{76}\text{Si}_3\text{Ti}_3$: C, 62.36; H, 9.47. Found: C, 62.02; H, 9.38.

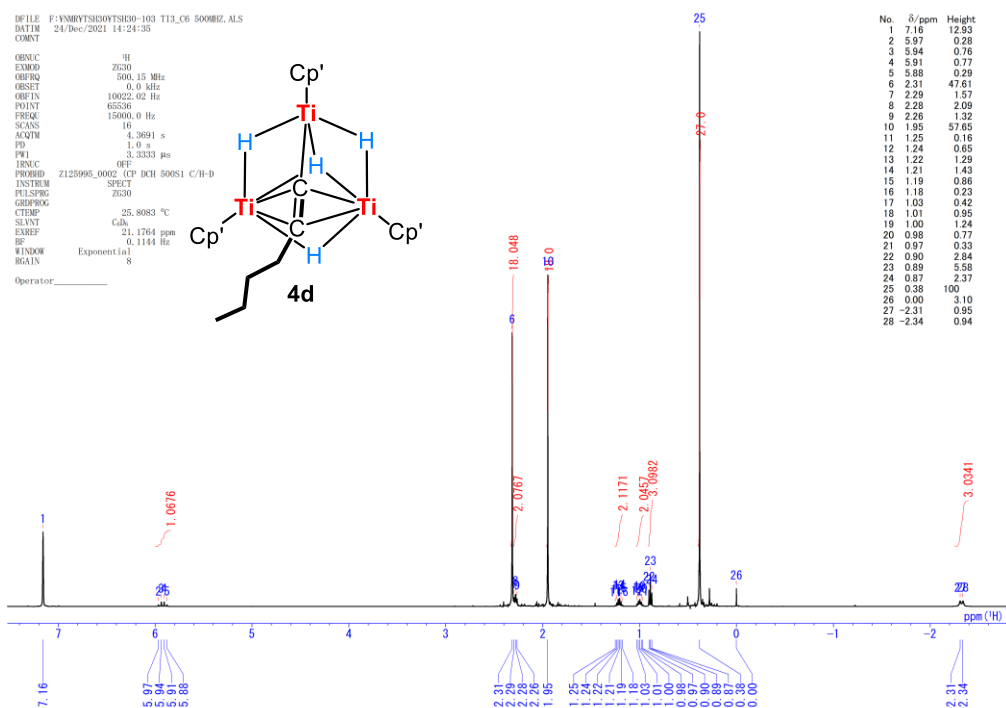


Figure S26. ¹H NMR spectrum of **4d** (C₆D₆, rt).

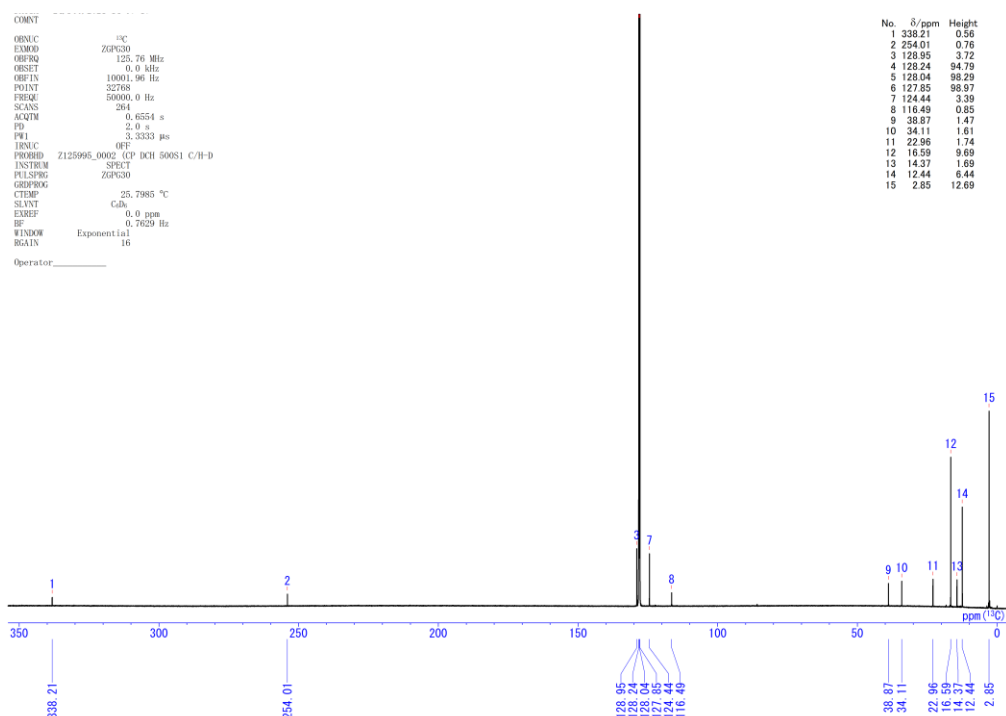


Figure S27. ¹³C{¹H} NMR spectrum of **4d** (C₆D₆, rt).

Reaction of 1 with styrene to yield 4e: [$\{(C_5Me_4SiMe_3)Ti\}_3(\mu_3-\eta^2:\eta^2:\eta^1-C=CPh)(\mu-H)_3(\mu_3-H)$] (**4e**). To a 1.0 mL hexane solution of **1** (47 mg, 0.064 mmol) was added styrene (25 μL, 0.22 mmol) in a sample tube in an Ar glovebox. The solution was kept at room temperature for 2 h. The solution turned from brown to dark red-brown. After removal of the solvent under vacuum, the oily crude product was crystallized in DME

at $-30\text{ }^{\circ}\text{C}$ to give dark brown solids of $[\{(C_5Me_4SiMe_3)Ti\}_3(\mu_3-\eta^2:\eta^2:\eta^1-C=CPh)(\mu-H)_3(\mu_3-H)]$ (**4e**) (28 mg, 0.034 mmol, 53%).

Characterization of 4e: 1H NMR (C_6D_6 , rt): δ 7.08 (t, $J = 7.6$ Hz, 2H, Ph), 6.82 (t, $J = 7.6$ Hz, 1H, Ph), 6.69 (d, $J = 7.6$ Hz, 2H, Ph), 5.38 (q, $J = 15.0$ Hz, 1H, μ_3-H), 2.37 (brs, 18H, $C_5Me_4SiMe_3$), 1.88 (brs, 18H, $C_5Me_4SiMe_3$), 0.34 (s, 27H, $C_5Me_4SiMe_3$), -2.75 (brs, 2~3H, $\mu-H$). 1H NMR (C_6D_6 , $50\text{ }^{\circ}\text{C}$): δ 7.08 (t, $J = 7.6$ Hz, 2H, Ph), 6.81 (t, $J = 7.6$ Hz, 1H, Ph), 6.68 (d, $J = 7.6$ Hz, 2H, Ph), 5.39 (brs, 1H, μ_3-H), 2.37 (s, 18H, $C_5Me_4SiMe_3$), 1.89 (brs, 18H, $C_5Me_4SiMe_3$), 0.34 (s, 27H, $C_5Me_4SiMe_3$), -1.73 (brs, 1~2H, $\mu-H$). 1H NMR (THF- d_8 , $-30\text{ }^{\circ}\text{C}$): δ 6.96 (brs, 2H, Ph), 6.73 (brs, 1H, Ph), 6.44 (brs, 2H, Ph), 5.21 (m, 1H, μ_3-H), 2.38 (s, 6H, $C_5Me_4SiMe_3$), 2.36 (s, 6H, $C_5Me_4SiMe_3$), 2.15 (s, 6H, $C_5Me_4SiMe_3$), 2.10 (s, 6H, $C_5Me_4SiMe_3$), 1.78 (s, 6H, $C_5Me_4SiMe_3$), 1.65 (s, 6H, $C_5Me_4SiMe_3$), 0.64 (d, $J = 17.8$ Hz, 1H, $\mu-H$), 0.19 (s, 27H, $C_5Me_4SiMe_3$), -3.09 (d, $J = 12.8$ Hz, 2H, $\mu-H$). $^{13}C\{^1H\}$ NMR (C_6D_6 , $60\text{ }^{\circ}\text{C}$): δ 341.1 (s, $\mu_3-C=CPh$), 245.8 (s, $\mu_3-C=CPh$), 145.7 (s, $\mu_3-C=CPh$), 129.6 (brs, $C_5Me_4SiMe_3$), 127.2 (s, $\mu_3-C=CPh$), 126.3 (s, $\mu_3-C=CPh$), 125.5 (brs, $C_5Me_4SiMe_3$), 124.9 (s, $\mu_3-C=CPh$), 118.4 (brs, $C_5Me_4SiMe_3$), 16.7 (s, $C_5Me_4SiMe_3$), 12.7 (s, $C_5Me_4SiMe_3$), 2.7 (s, $C_5Me_4SiMe_3$). Anal. calcd. for $C_{44}H_{72}Si_3Ti_3$: C, 63.76; H, 8.76. Found: C, 63.15; H, 8.76.

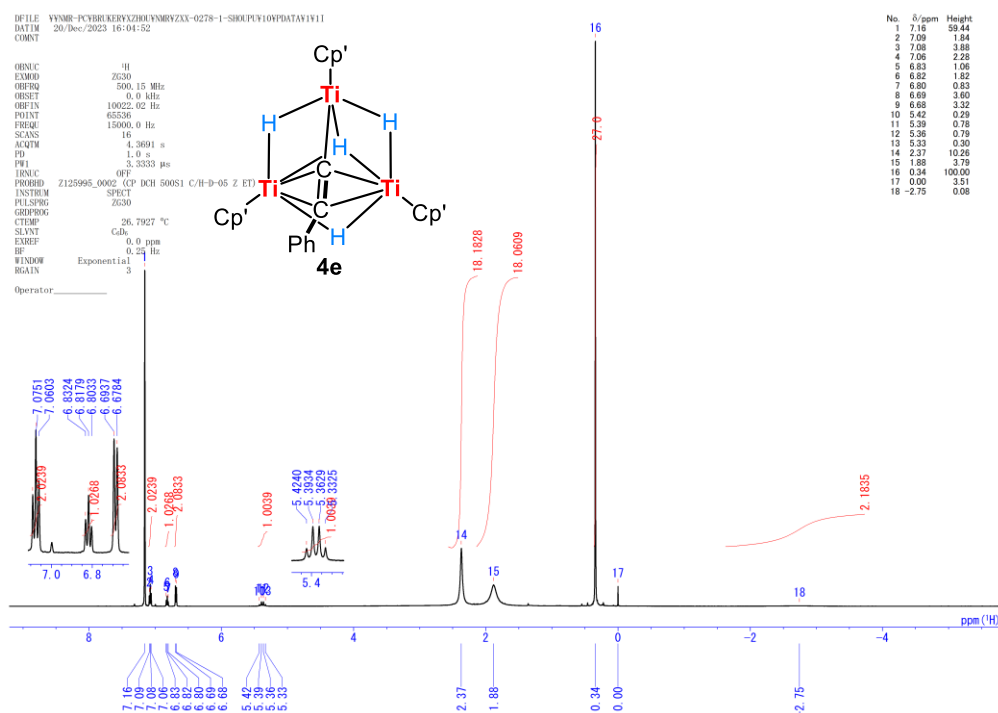


Figure S28. 1H NMR spectrum of **4e** (C_6D_6 , rt).

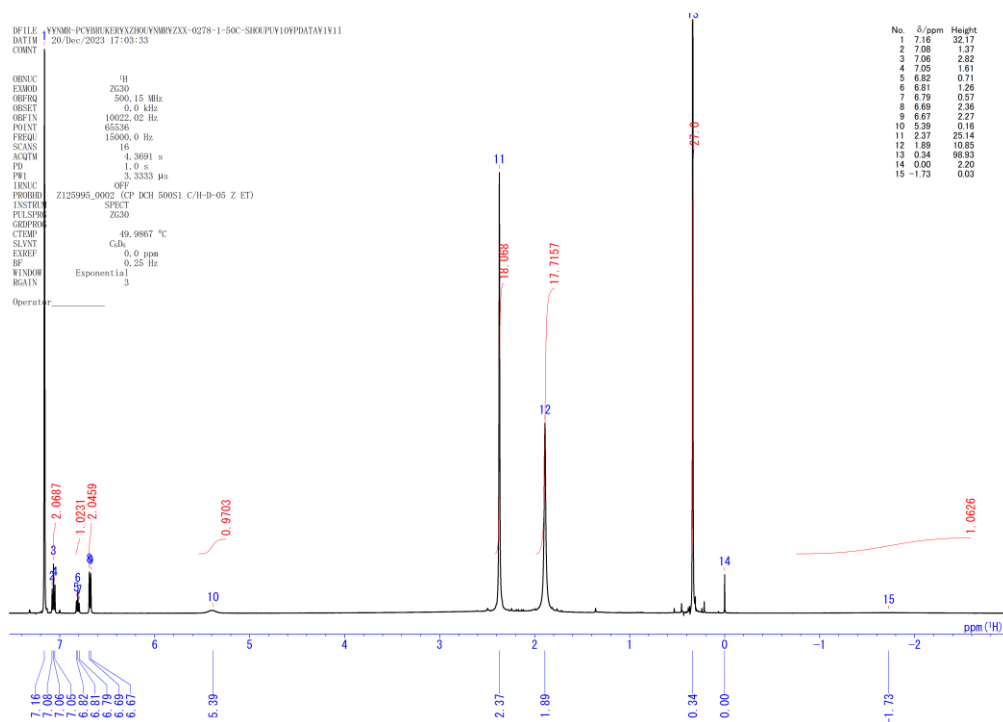


Figure S29. ¹H NMR spectrum of **4e** (C₆D₆, 50 °C).

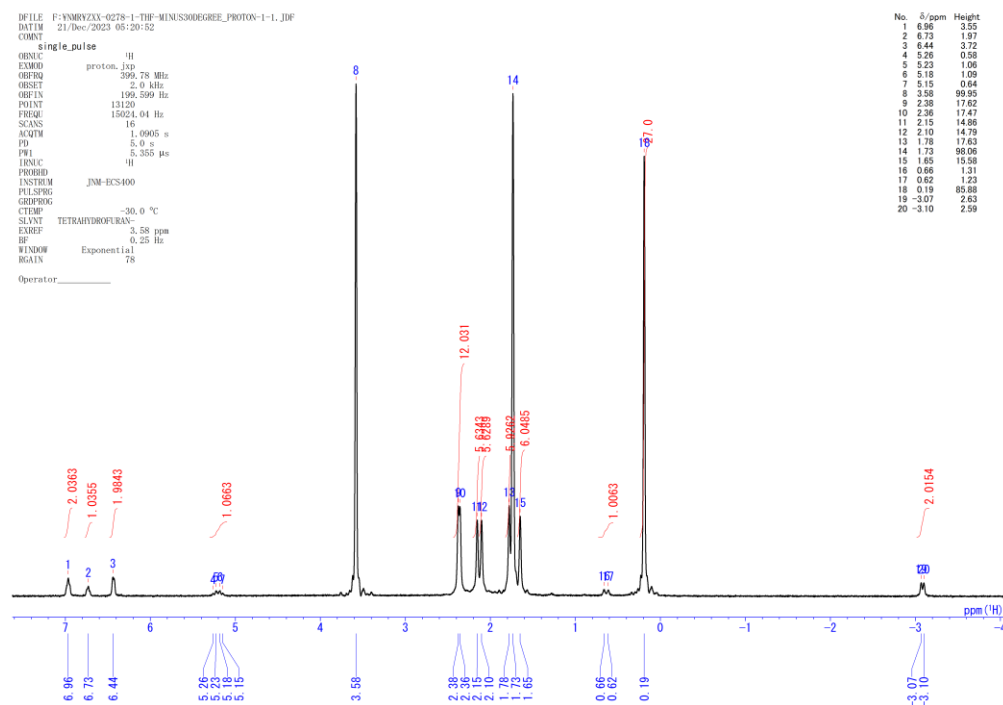


Figure S30. ¹H NMR spectrum of **4e** (THF-*d*₈, -30 °C).

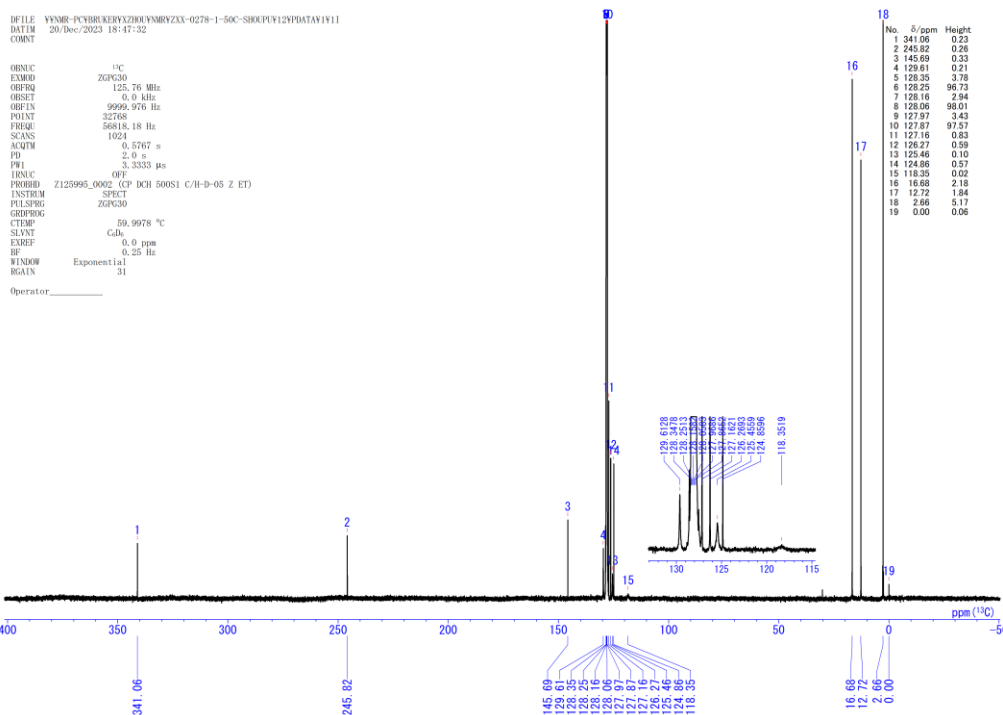


Figure S31. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4e** (C_6D_6 , 60 °C).

Reaction of 1 with norbornene to yield 4f: To a 3.0 mL hexane solution of **1** (110 mg, 0.15 mmol) was added norbornene (42 mg, 0.45 mmol) in a sample tube in an Ar glovebox. The solution was kept at room temperature for 2 h. After removal of the solvent under vacuum, the crude product was crystallized in DME at $-30\text{ }^\circ\text{C}$ to give dark brown-purple solids of $[\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-}\eta^2\text{:}\eta^2\text{:}\eta^1\text{-C=CC}_5\text{H}_9)(\mu\text{-H})_3(\mu_3\text{-H})]$ (**4f**) (80 mg, 0.097 mmol, 65%).

Characterization of 4f: ^1H NMR (C_6D_6 , rt): δ 4.02 (q, $J = 14.3$ Hz, 1H, $\mu_3\text{-H}$), 2.65 (qt, $J = 7.6$ Hz, 1H, $\text{-C}_5\text{H}_9$), 2.32 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 1.99 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 1.67 (m, 2H, $\text{-C}_5\text{H}_9$), 1.59 (m, 2H, $\text{-C}_5\text{H}_9$), 1.41 (m, 2H, $\text{-C}_5\text{H}_9$), 0.94 (m, 2H, $\text{-C}_5\text{H}_9$), 0.37 (s, 27H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), -2.44 (d, $J = 14.3$ Hz, 3H, $\mu\text{-H}$). $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , rt): δ 341.0 (s, $\mu_3\text{-C=CC}_5\text{H}_9$), 255.6 (s, $\mu_3\text{-C=CC}_5\text{H}_9$), 129.4 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 124.6 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 116.6 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 49.5 (s, $\mu_3\text{-C=CC}_5\text{H}_9$), 37.6 (s, $\mu_3\text{-C=CC}_5\text{H}_9$), 25.7 (s, $\mu_3\text{-C=CC}_5\text{H}_9$), 16.9 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 12.9 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 3.0 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$). Anal. calcd. for $\text{C}_{43}\text{H}_{76}\text{Si}_3\text{Ti}_3$: C, 62.91; H, 9.33. Found: C, 61.85; H, 9.32.

Preparation of 4f': The $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$ -ligated complex $[\{(\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu})\text{Ti}\}_3(\mu_3\text{-}\eta^2\text{:}\eta^2\text{:}\eta^1\text{-C=CC}_5\text{H}_9)(\mu\text{-H})_3(\mu_3\text{-H})]$ (**4f'**) was prepared in a manner identical to that for **4f** using $[\{(\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu})\text{Ti}\}_3(\mu_3\text{-H})(\mu\text{-H})_6]$ (**1'**) and norbornene as starting materials. Single crystals of **4f'** suitable for X-ray diffraction studies were obtained by recrystallization from a DME/benzene solution at $-30\text{ }^\circ\text{C}$.

Characterization of 4f': ^1H NMR (C_6D_6 , rt): δ 4.25 (q, $J = 14.3$ Hz, 1H, $\mu_3\text{-H}$), 2.62 (qt, $J = 7.8$ Hz, 1H, $\text{-C}_5\text{H}_9$), 2.36 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 2.01 (s, 18H,

$C_5Me_4SiMe_2^tBu$), 1.76 (m, 2H, $-C_5H_9$), 1.66 (m, 2H, $-C_5H_9$), 1.43 (m, 2H, $-C_5H_9$), 1.10 (s, 27H, $C_5Me_4SiMe_2^tBu$), 0.99 (m, 2H, $-C_5H_9$), 0.34 (s, 18H, $C_5Me_4SiMe_2^tBu$), -2.39 (d, $J = 14.3$ Hz, 3H, $\mu-H$). $^{13}C\{^1H\}$ NMR (C_6D_6 , rt): δ 340.4 (s, $\mu_3-C=CC_5H_9$), 256.0 (s, $\mu_3-C=CC_5H_9$), 130.0 (s, $C_5Me_4SiMe_2^tBu$), 125.0 (s, $C_5Me_4SiMe_2^tBu$), 115.1 (s, $C_5Me_4SiMe_2^tBu$), 49.8 (s, $\mu_3-C=CC_5H_9$), 38.0 (s, $\mu_3-C=CC_5H_9$), 27.7 (s, $C_5Me_4SiMe_2^tBu$), 25.8 (s, $\mu_3-C=CC_5H_9$), 20.2 (s, $C_5Me_4SiMe_2^tBu$), 17.2 (s, $C_5Me_4SiMe_2^tBu$), 13.0 (s, $C_5Me_4SiMe_2^tBu$), -0.1 (s, $C_5Me_4SiMe_2^tBu$).

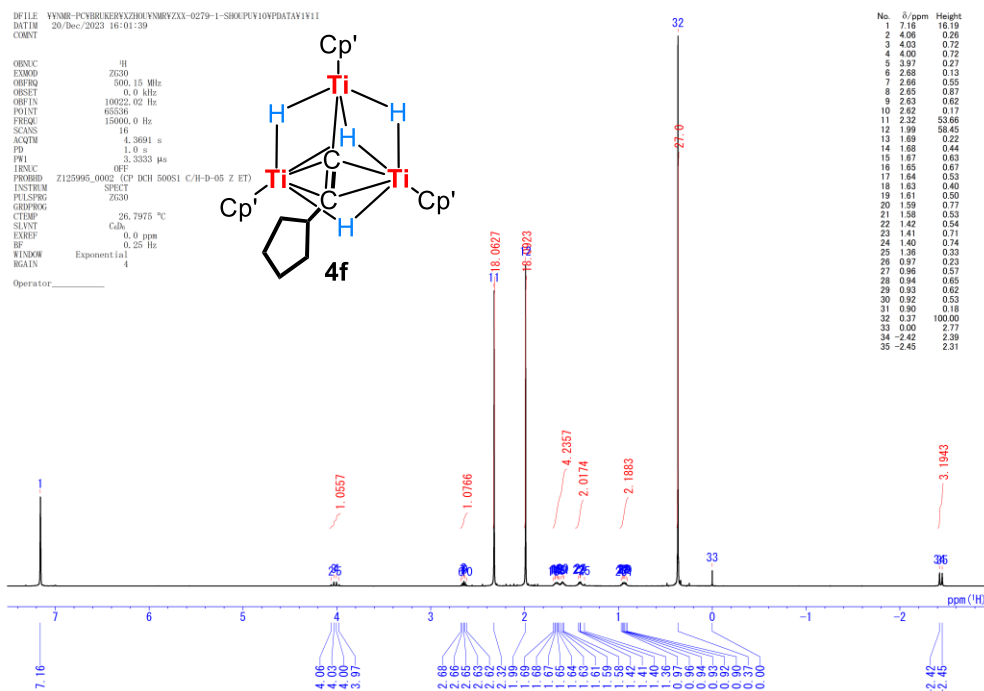


Figure S32. 1H NMR spectrum of **4f** (C_6D_6 , rt).

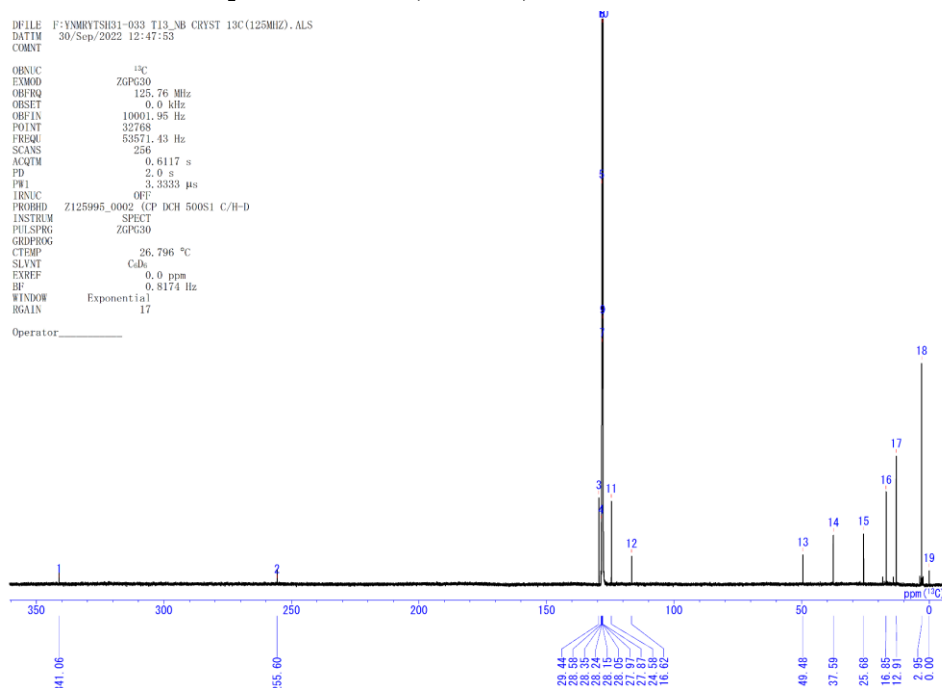


Figure S33. $^{13}C\{^1H\}$ NMR spectrum of **4f** (C_6D_6 , rt).

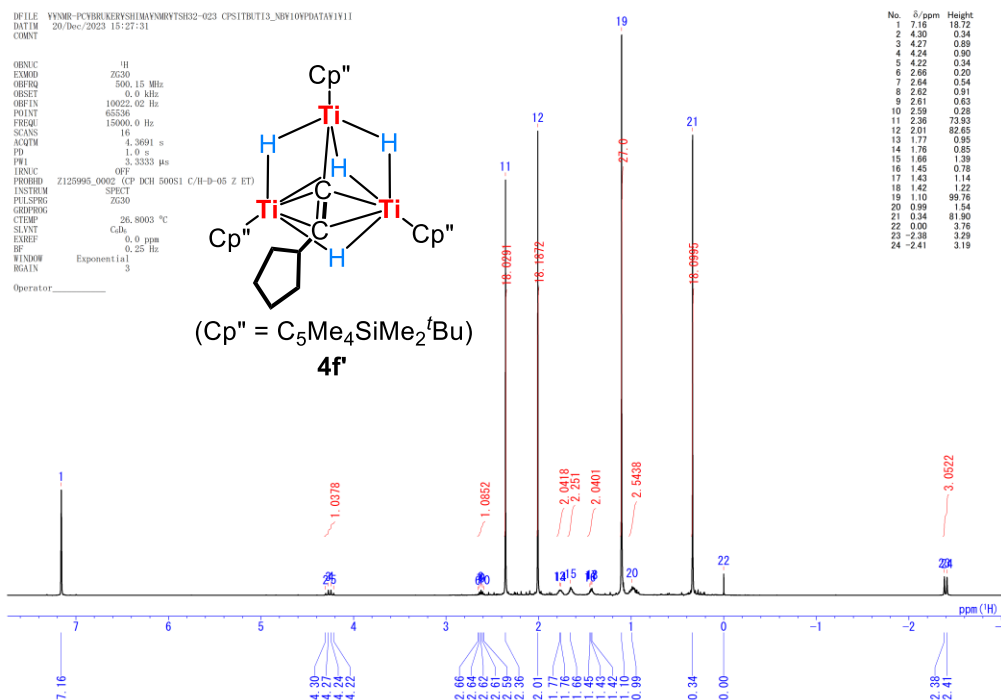


Figure S34. ¹H NMR spectrum of **4f'** (C₆D₆, rt).

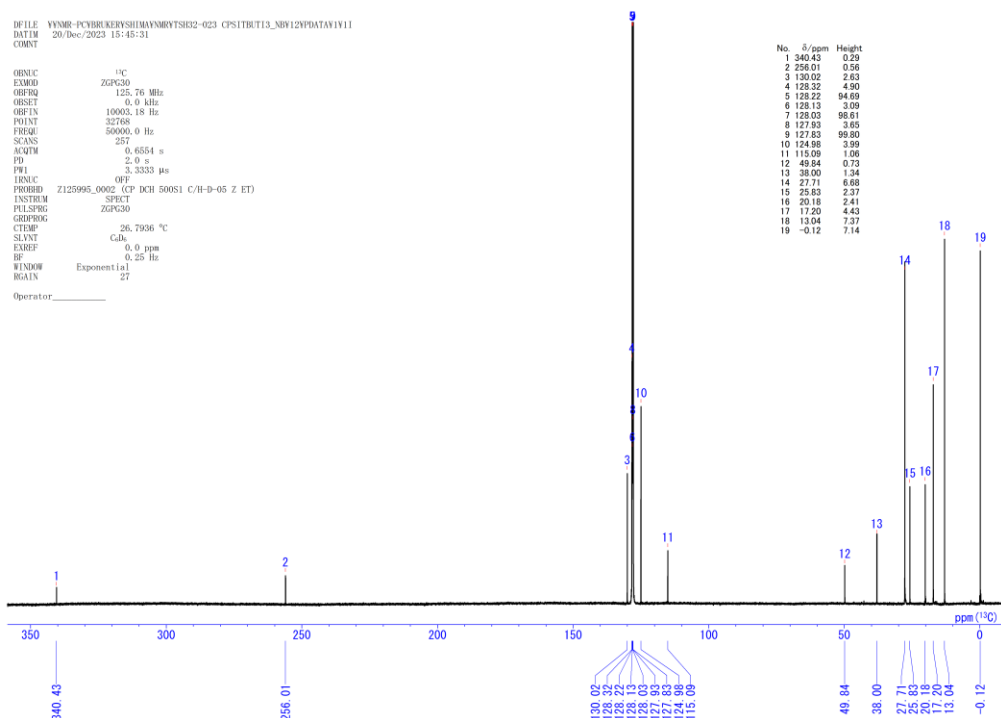


Figure S35. ¹³C{¹H} NMR spectrum of **4f'** (C₆D₆, rt).

Reaction of 1 with cyclohexene to yield 4g: To a 2.0 mL hexane solution of **1** (66 mg, 0.090 mmol) was added cyclohexene (100 μL, 1 mmol) in 50 mL Schlenk tube equipped with a J. Young valve. The solution was kept at 60 °C for 2 days. The solution turned from brown to dark red-brown. After removal of the solvent under vacuum, the oily crude product was crystallized in DME at −30 °C to give dark brown solids of [$\{(C_5Me_4SiMe_3)Ti\}_3(\mu_3-\eta^2:\eta^2:\eta^2-C_6H_7)(\mu-H)_3(\mu_3-H)$] (**4g**) (44 mg, 0.055 mmol, 61%).

Single crystals of **4g** suitable for X-ray diffraction studies were obtained by recrystallization from a DME/benzene solution at $-30\text{ }^{\circ}\text{C}$.

Reaction of 1 with 1,3-cyclohexadiene to yield 4g: To a 3.0 mL hexane solution of **1** (72 mg, 0.099 mmol) was added 1,3-cyclohexadiene (40 μL , 0.42 mmol) in a sample tube in an Ar glovebox. The solution was kept at room temperature for 2 days. After removal of the solvent under vacuum, the oily crude product was crystallized in DME at $-30\text{ }^{\circ}\text{C}$ to give dark brown solids of $[\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-}\eta^2\text{:}\eta^2\text{:}\eta^2\text{-C}_6\text{H}_7)(\mu\text{-H})_3(\mu_3\text{-H})]$ (**4g**) (48 mg, 0.059 mmol, 60%).

Characterization of 4g: ^1H NMR (C_6D_6 , rt, tentative): δ 3.28 (brs, 1~2H, $\text{-CH}_2\text{-}$), 2.56 (q, $J = 13.4\text{ Hz}$, 1H, $\mu_3\text{-H}$), 2.21 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 2.03 (brs, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 1.81 (t, $J = 6.1\text{ Hz}$, 1H, -CH-), 1.12 (brs, ~4H, $\text{-CH}_2\text{-}$ and $\mu\text{-H}$), 0.36 (s, 27H, $\text{C}_5\text{Me}_4\text{SiMe}_3$). ^1H NMR (C_6D_6 , $50\text{ }^{\circ}\text{C}$): δ 3.26 (brs, 2H, $\text{-CH}_2\text{-}$), 2.56 (q, $J = 13.4\text{ Hz}$, 1H, $\mu_3\text{-H}$), 2.21 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 2.03 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 1.82 (t, $J = 6.1\text{ Hz}$, 1H, -CH-), 1.10 (brs, 7H, $\text{-CH}_2\text{-}$ and $\mu\text{-H}$), 0.35 (s, 27H, $\text{C}_5\text{Me}_4\text{SiMe}_3$). $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , rt): δ 245.7 (s, $\mu_3\text{-C}$ or $\mu\text{-C}$), 216.2 (s, $\mu_3\text{-C}$ or $\mu\text{-C}$), 127.6 (brs, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 123.6 (brs, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 114.4 (brs, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 97.9 (s, -CH-), 38.3 (s, $\text{-CH}_2\text{-}$), 32.2 (s, $\text{-CH}_2\text{-}$), 25.4 (s, $\text{-CH}_2\text{-}$), 16.5 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 12.6 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 2.8 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$). Anal. calcd. for $\text{C}_{42}\text{H}_{74}\text{Si}_3\text{Ti}_3$: C, 62.52; H, 9.24. Found: C, 61.83; H, 9.01.

The reaction of **1** with a conjugated diene such as 1,3-butadiene gave a complicated mixture.

Preparation of 4g': The $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$ -ligated complex $[\{(\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu})\text{Ti}\}_3(\mu_3\text{-}\eta^2\text{:}\eta^2\text{:}\eta^2\text{-C}_6\text{H}_7)(\mu\text{-H})_3(\mu_3\text{-H})]$ (**4g'**) was prepared in a manner identical to that for **4g** using $[\{(\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu})\text{Ti}\}_3(\mu_3\text{-H})(\mu\text{-H})_6]$ (**1'**) and 1,3-cyclohexadiene as starting materials.

Characterization of 4g': ^1H NMR (C_6D_6 , rt, tentative): δ 3.29 (brs, 1~2H, $\text{-CH}_2\text{-}$), 2.40 (q, $J = 13.3\text{ Hz}$, 1H, $\mu_3\text{-H}$), 2.28 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 2.05 (brs, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 1.86 (brs, 1H, -CH-), 1.16 (brs, ~2H, $\text{-CH}_2\text{-}$ and $\mu\text{-H}$), 1.04 (s, 27H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 0.37 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$). ^1H NMR (C_6D_6 , $60\text{ }^{\circ}\text{C}$): δ 3.28 (brs, 2H, $\text{-CH}_2\text{-}$), 2.45 (q, $J = 13.3\text{ Hz}$, 1H, $\mu_3\text{-H}$), 2.28 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 2.06 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 1.88 (brs, 1H, -CH-), 1.15 (brs, 4H, $\text{-CH}_2\text{-}$), 1.02 (s, 27H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 0.37 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$). $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , rt): δ 246.7 (s, $\mu_3\text{-C}$ or $\mu\text{-C}$), 216.4 (s, $\mu_3\text{-C}$ or $\mu\text{-C}$), 127.5 (brs, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 124.1 (brs, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 112.3 (brs, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 97.9 (s, -CH-), 37.8 (s, $\text{-CH}_2\text{-}$), 32.7 (s, $\text{-CH}_2\text{-}$), 27.6 (s, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 25.4 (s, $\text{-CH}_2\text{-}$), 20.3 (s, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 16.9 (s, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 13.0 (s, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), -0.6 (s, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$).

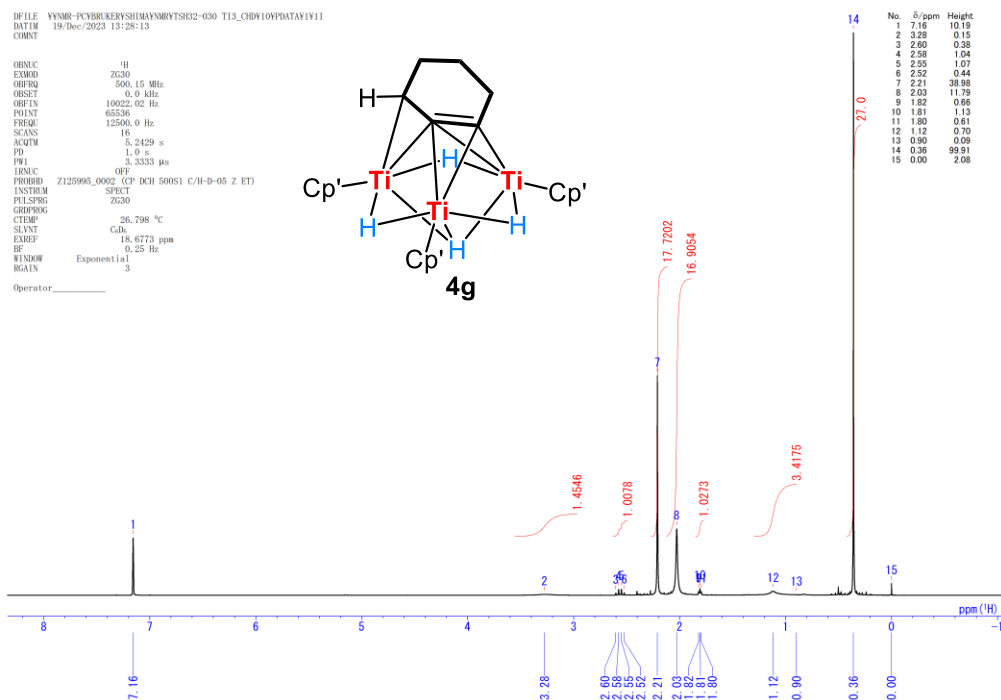


Figure S36. ¹H NMR spectrum of **4g** (C₆D₆, rt).

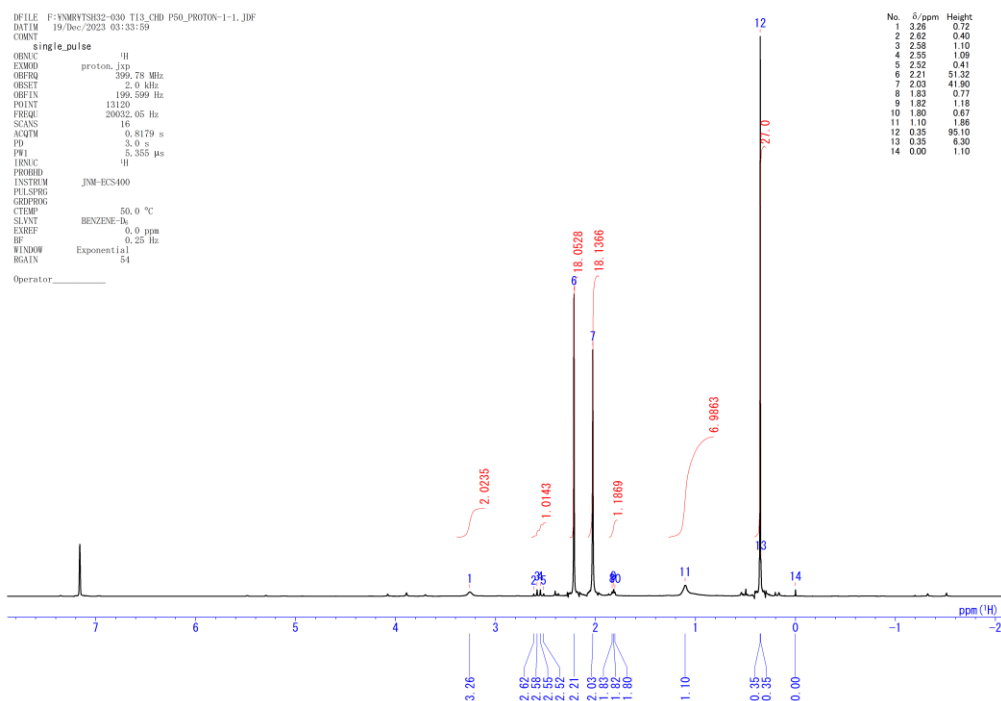


Figure S37. ¹H NMR spectrum of **4g** (C₆D₆, 50 °C).

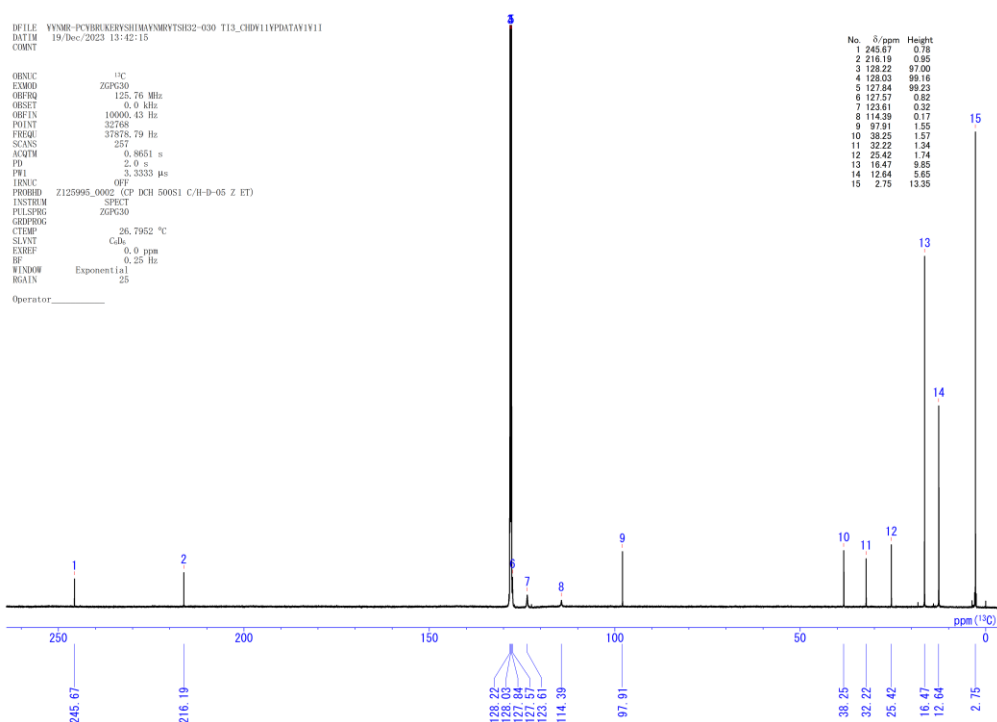


Figure S38. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **4g** (C_6D_6 , rt).

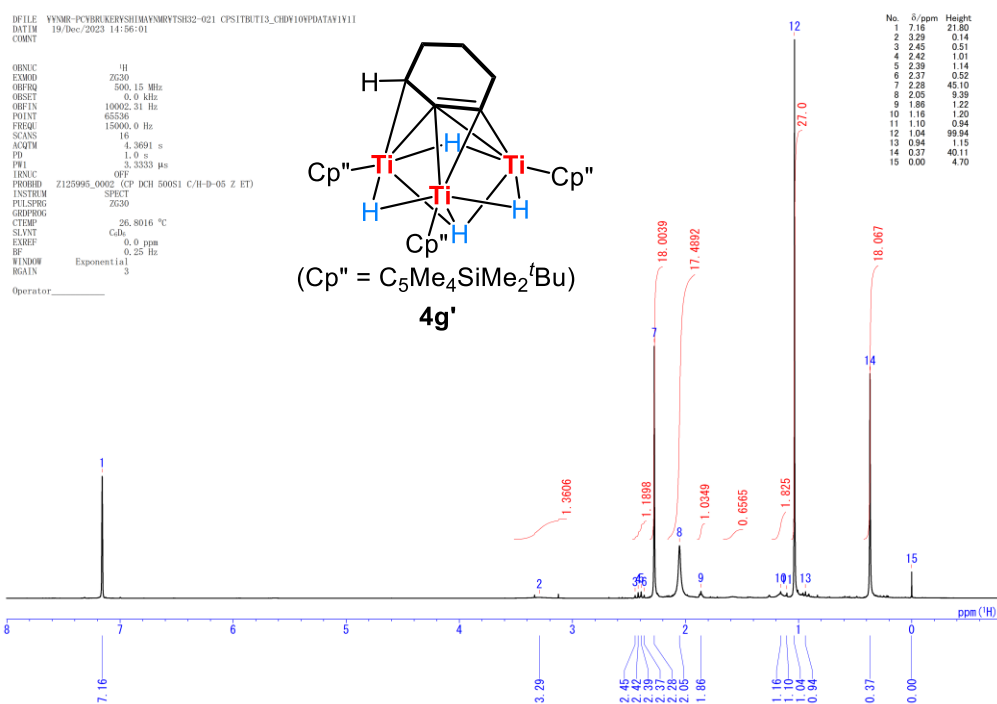


Figure S39. ^1H NMR spectrum of **4g'** (C_6D_6 , rt).

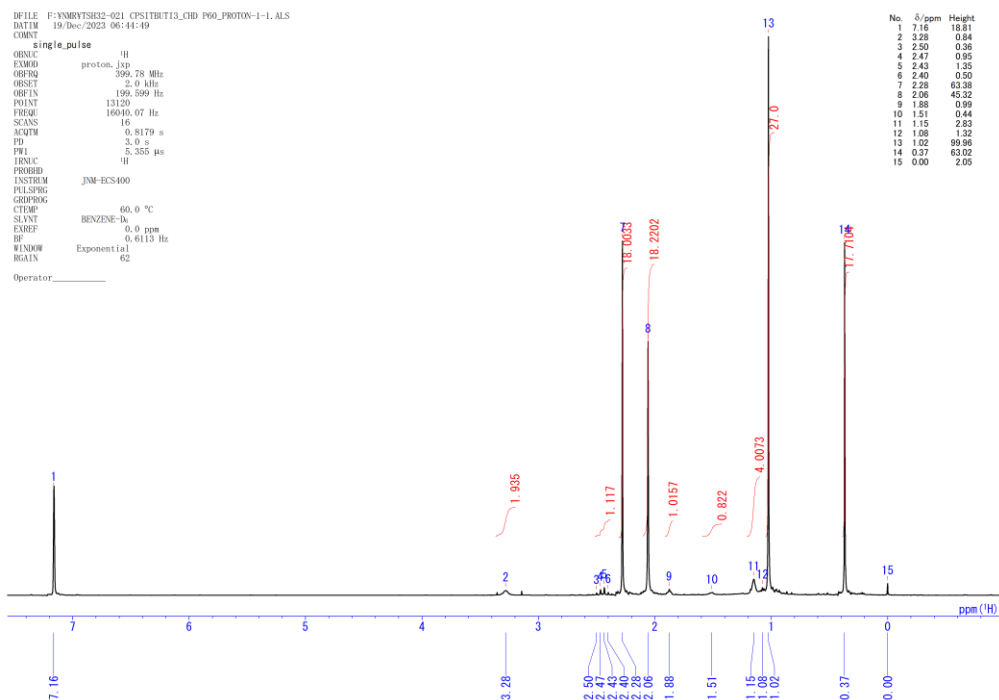


Figure S40. ¹H NMR spectrum of **4g'** (C₆D₆, 60 °C).

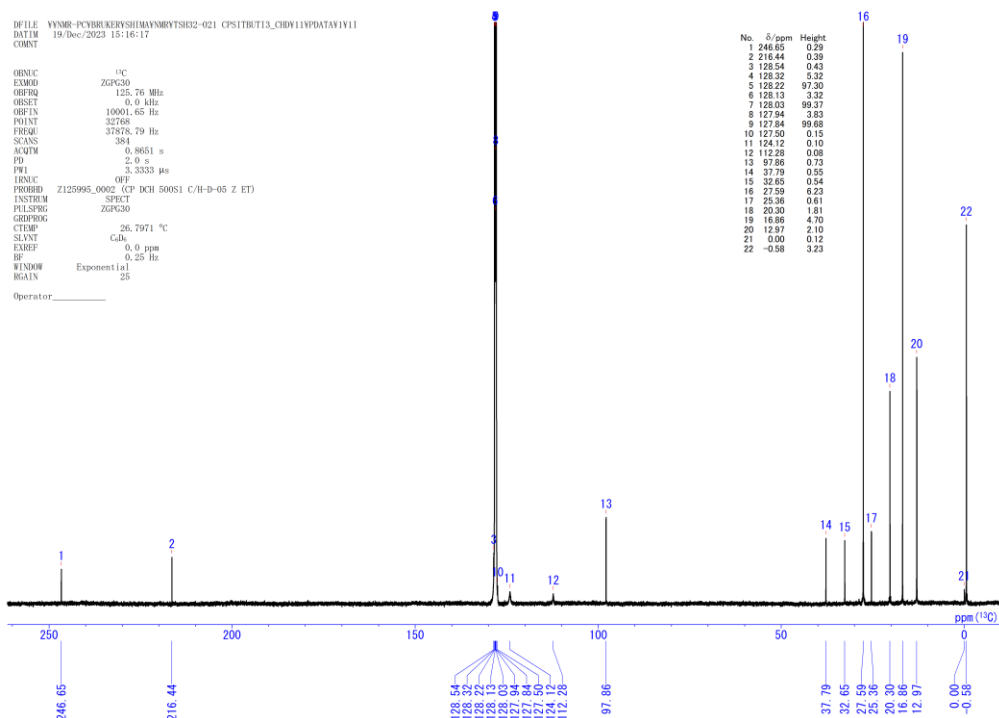


Figure S41. ¹³C{¹H} NMR spectrum of **4g'** (C₆D₆, rt).

Reaction of 4a with N₂ (10 atm) to yield 5: A hexane solution (2.0 mL) of **4a** (41 mg, 0.053 mmol) in 10 mL Hiper Glass Cylinder (TAIATSU TECHNO[®]) was filled with 10 atm of N₂. The solution was stirred at room temperature for 2 days. The color of the solution changed from dark brown to dark purple. After the reaction, the solution was evaporated and the residue was crystallized in DME at −30 °C to give [$\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-}\eta^3\text{:}\eta^3\text{:}\eta^1\text{-CH=C(CH}_3\text{)N-})(\mu_3\text{-N})(\mu\text{-H})$] (**5**). (37 mg, 0.047 mmol,

89%) as dark-purple solid. Single crystals suitable for X-ray diffraction study were obtained from the concentrated DME/C₆H₆ solution of **5** at -30 °C.

Characterization of 5: ¹H NMR (C₆D₆, rt): δ 7.53 (d, *J*_{HH} = 1.2 Hz, 1H, =CH-), 2.89 (s, 3H, C₅Me₄SiMe₃ or Me), 2.58 (s, 3H, C₅Me₄SiMe₃ or Me), 2.54 (s, 3H, C₅Me₄SiMe₃ or Me), 2.45 (s, 1H, μ-H), 2.44 (s, 3H, C₅Me₄SiMe₃ or Me), 2.29 (s, 3H, C₅Me₄SiMe₃ or Me), 2.26 (s, 3H, C₅Me₄SiMe₃ or Me), 2.17₃ (s, 3H, C₅Me₄SiMe₃ or Me), 2.16₉ (s, 3H, C₅Me₄SiMe₃ or Me), 2.05 (s, 3H, C₅Me₄SiMe₃ or Me), 1.80 (s, 3H, C₅Me₄SiMe₃ or Me), 1.63 (s, 3H, C₅Me₄SiMe₃ or Me), 1.54 (s, 3H, C₅Me₄SiMe₃), 1.53 (s, 3H, C₅Me₄SiMe₃), 0.28 (s, 9H, C₅Me₄SiMe₃), 0.16 (s, 9H, C₅Me₄SiMe₃), 0.15 (s, 9H, C₅Me₄SiMe₃). ¹³C{¹H} NMR (C₆D₆, rt): δ 191.8 (s, -CH=C(N)CH₃), 130.8, 130.4, 129.9, 126.4, 126.33, 126.27, 126.24, 126.0, 125.4 (s, C₅Me₄SiMe₃), 124.5 (s, -CH=C(N)CH₃), 122.7, 122.3, 122.2, 117.4, 116.6, 115.7 (s, C₅Me₄SiMe₃), 27.1 (s, -CH=C(N)CH₃), 17.3, 17.0, 16.22, 16.20, 16.0, 15.4, 13.2, 12.8, 12.4, 11.9, 11.7, 11.5 (s, C₅Me₄SiMe₃), 2.36, 2.28, 2.26 (s, C₅Me₄SiMe₃). IR (KBr, Nujol mulls, cm⁻¹): 2959 (vs), 2911 (vs), 2853 (vs), 1455 (s), 1374 (s), 1325 (s), 1287 (m), 1246 (s), 1213 (w), 1130 (s), 1085 (w), 1024 (s), 947 (w), 835 (vs), 754 (s), 683 (s), 632 (s), 546 (s), 520 (s), 502 (s). Anal. calcd. for C₃₉H₆₈N₂Si₃Ti₃: C, 59.08; H, 8.64; N, 3.53. Found: C, 58.81; H, 8.80; N, 2.98.

Formation and characterization of ¹⁵N-labelled 5-¹⁵N: A J. Young valve NMR sample tube was charged with C₆D₆ (0.4 mL) and complex **4a** (11 mg, 0.014 mmol). The solution was frozen in liquid nitrogen, degassed and ¹⁵N₂ gas (1 atm) was added. The solution was kept at room temperature for 4 days, yielding [{(C₅Me₄SiMe₃)Ti}₃(μ₃-η³:η³:η¹-CH=C(CH₃)¹⁵N-)(μ₃-¹⁵N)(μ-H)] (**5-¹⁵N**) in 87% NMR yield.

Characterization of 5-¹⁵N: ¹³C{¹H} NMR (C₆D₆, rt): δ 191.7 (s, C_α), 124.5 (d, *J*_{15NC} = 15.0 Hz, C_β), 27.1 (d, *J*_{15NC} = 5.3 Hz, Me). ¹⁵N{¹H} NMR (C₆D₆, rt): δ 431.3 (s, μ₃-¹⁵N), 177.2 (s, μ-¹⁵N-C). IR (KBr, Nujol mulls, cm⁻¹): 3952 (vs), 2917 (vs), 2852 (vs), 1456 (s), 1375 (s), 1326 (s), 1246 (s), 1212 (w), 1130 (m), 1084 (w), 1024 (s), 946 (w), 825 (vs), 754 (s), 687 (s), 632 (s), 551 (s), 519 (s).

The ¹⁵N{¹H} NMR spectrum of **5-¹⁵N** showed two sharp signals at δ_N 431.3 and 177.2, which are assignable to the nitride (μ₃-N) and imide (μ-N) units, respectively. In the ¹³C{¹H} NMR spectrum of **5-¹⁵N**, the doublet signal of the carbon bonding to the imide nitrogen was observed at δ_C 124.5 (d, *J*_{15NC} = 15.0 Hz), due to the coupling with the ¹⁵N atom (Fig. S44). In the ¹H NMR spectrum of **5**, the propenyl α-proton (Ti-CH=C(CH₃)-N) was observed at δ_H 7.53 (1H).

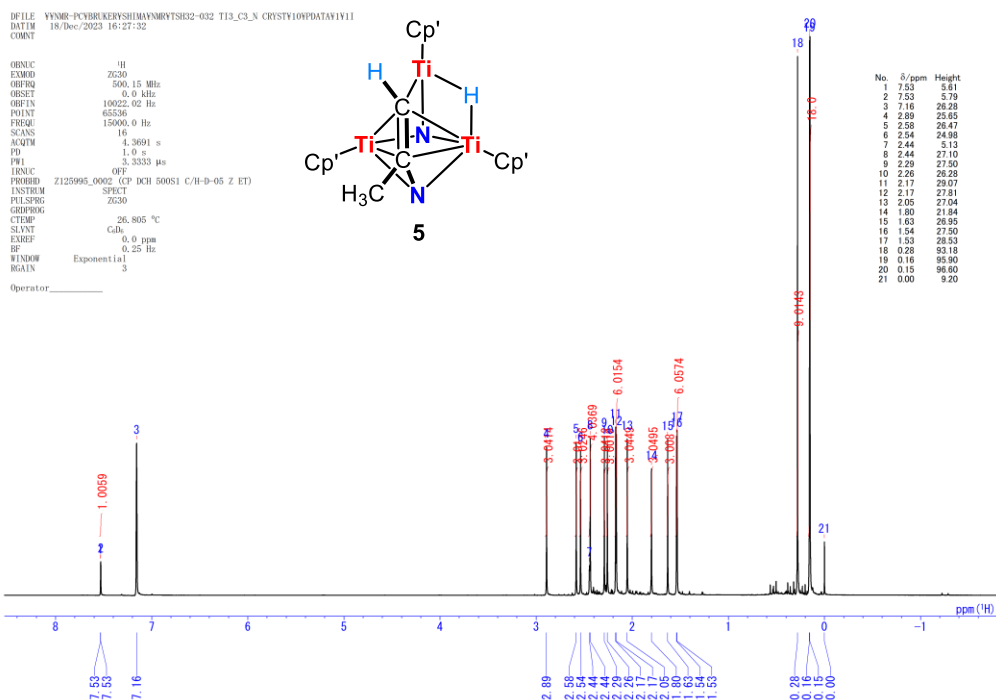
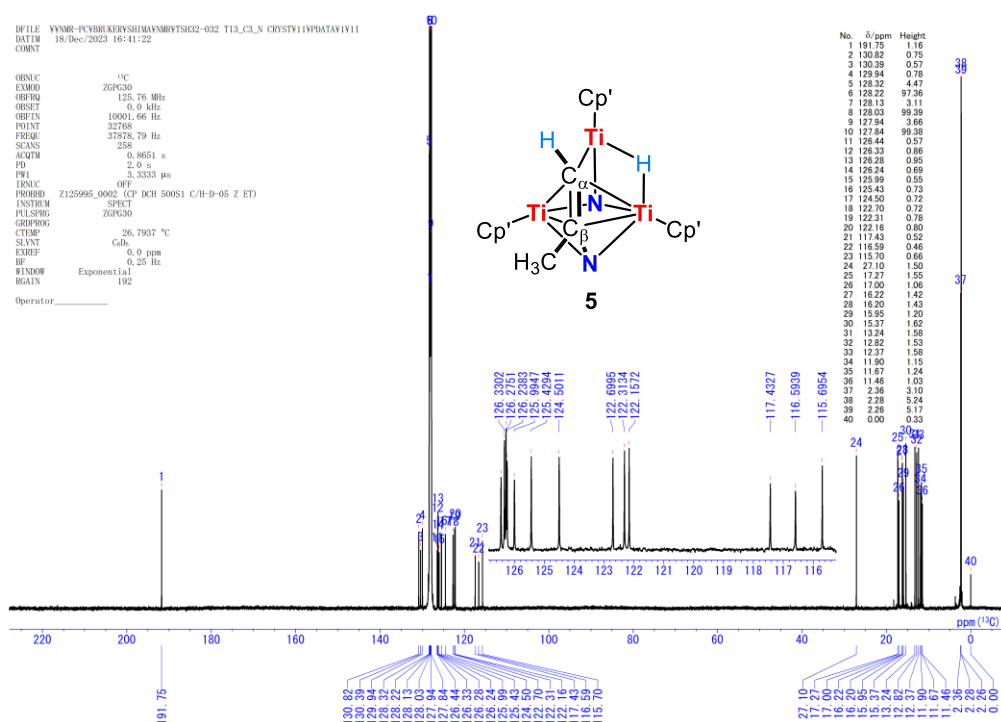


Figure S42. ¹H NMR spectrum of 5 (C₆D₆, rt).



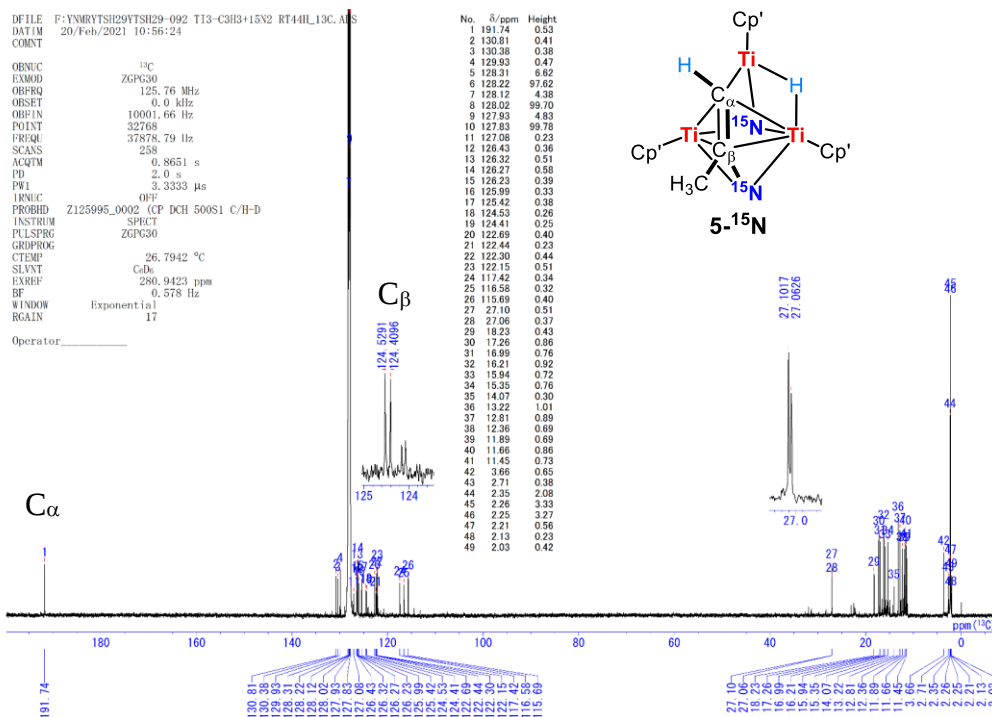


Figure S44. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $5\text{-}^{15}\text{N}$ (C_6D_6 , rt).

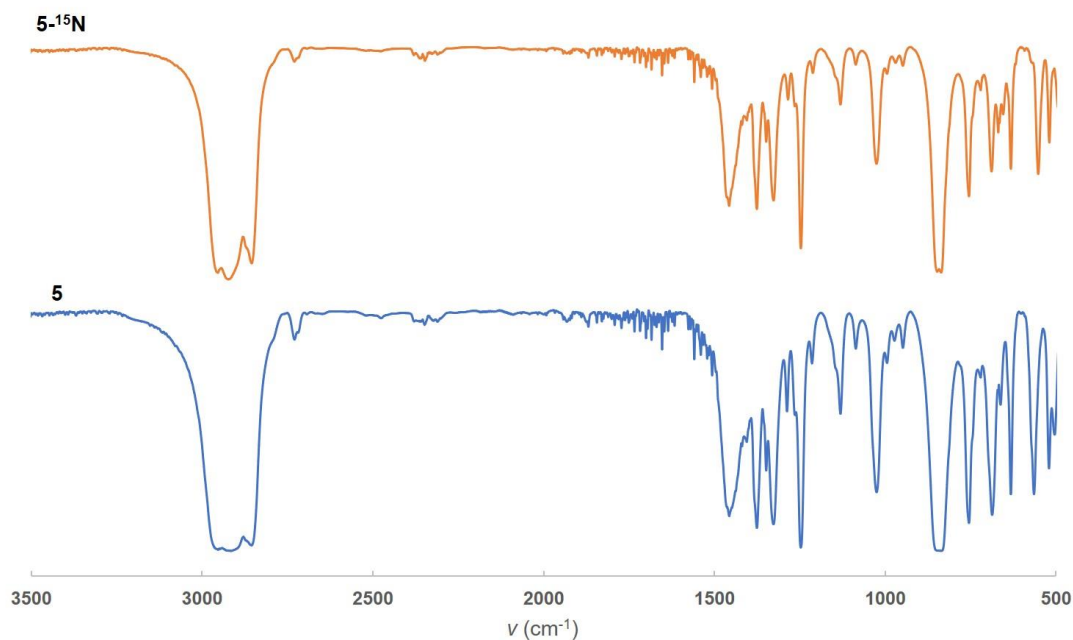


Figure S45. Stacked IR spectra of **5** and $5\text{-}^{15}\text{N}$.

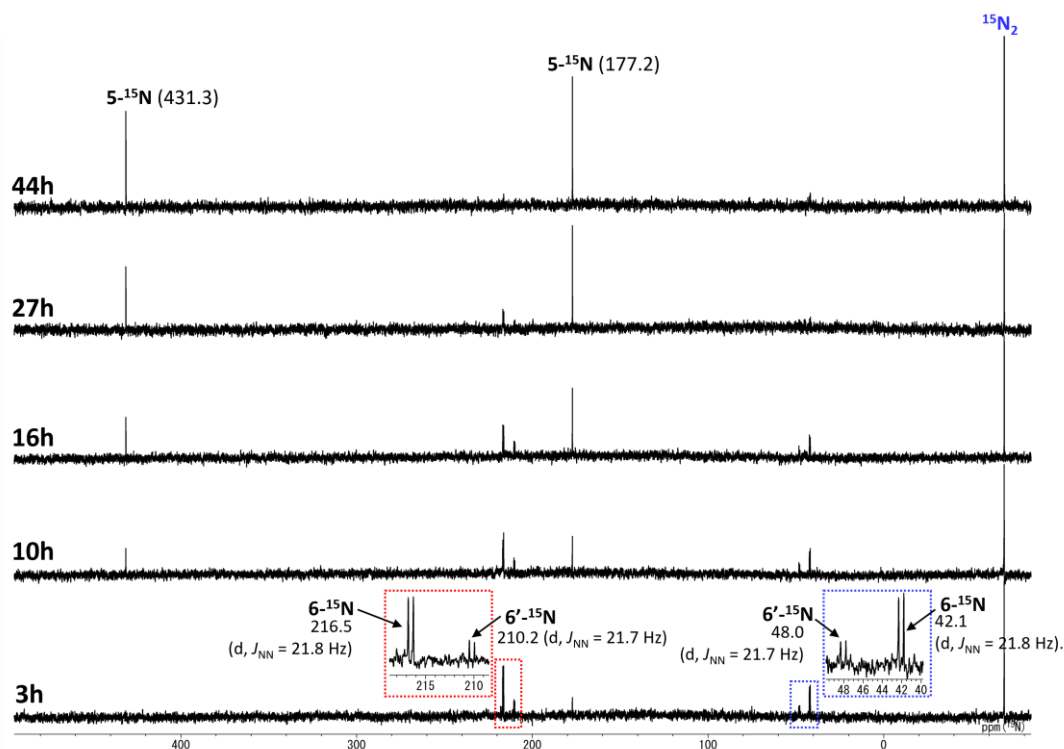
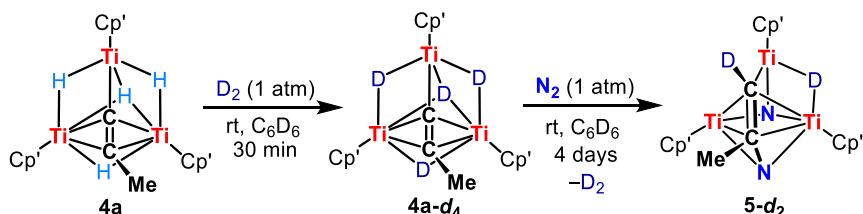


Figure S46. $^{15}\text{N}\{^1\text{H}\}$ NMR monitoring of the reaction of **4a** with $^{15}\text{N}_2$ in C_6D_6 (rt).

Reaction of deuterium-labelled **4a-d₄ with N_2 (1 atm) to yield deuterium-labelled **5-d₂**:**



A J. Young valve NMR sample tube was charged with 0.4 mL of C_6D_6 and complex **4a** (6 mg). The solution was frozen in liquid nitrogen, degassed and 1 atm of D_2 gas was added. The solution was kept at room temperature for 30 min and the ^1H NMR monitoring showed quantitative formation of the deuterated complex $[\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-}\eta^2\text{:}\eta^2\text{:}\eta^1\text{-C=CCH}_3)(\mu\text{-D})_3(\mu_3\text{-D})]$ (**4a-d₄**). After the confirmation of the deuteration, the solution was frozen in liquid nitrogen, degassed and 1 atm of N_2 gas was added. The reaction was monitored at room temperature by ^1H NMR. After 4 days, the partially deuterated complex $[\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-}\eta^3\text{:}\eta^3\text{:}\eta^1\text{-CD=C(CH}_3\text{)N-})(\mu_3\text{-N})(\mu\text{-D})]$ (**5-d₂**) was obtained, suggesting that hydride transfer to the propenylidene α -carbon in **4a** took place during the reaction.

Characterization of **5-d₂:** ^2H NMR (C_6H_6 , rt): δ 7.6 (s, $\text{C}_\alpha\text{-D}$), 2.4 (s, $\mu\text{-D}$).

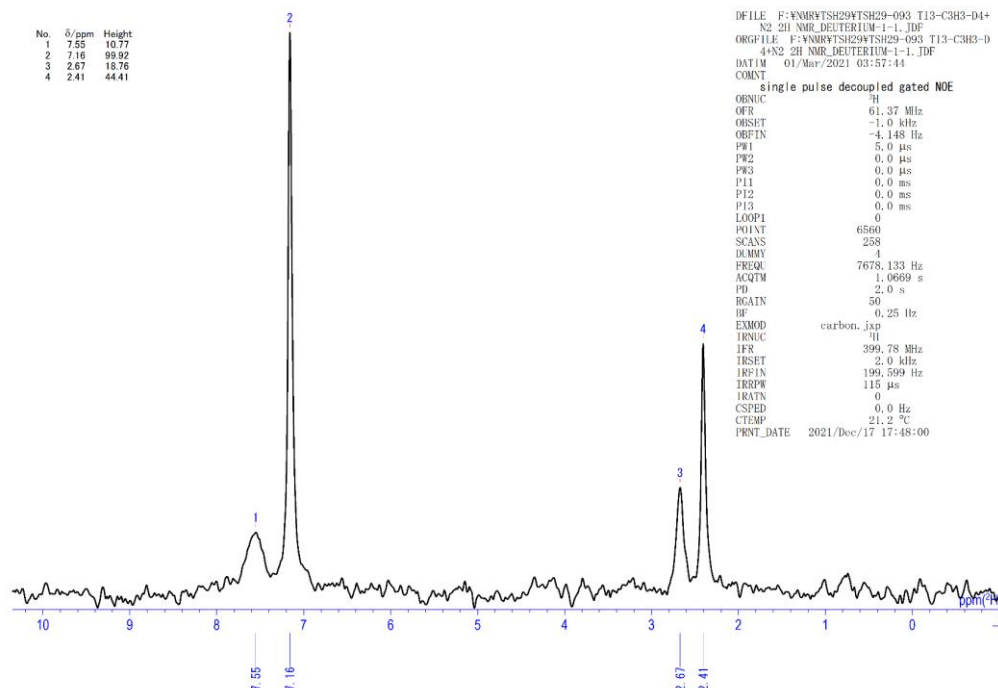


Figure S47. ^2H NMR spectrum of **5-d₂** (C_6H_6 , rt, the signal at δ_{H} 2.7 was derived from the byproduct **8a-d**).

Reaction of 4a with N_2 (1 or 5 atm) at -30°C to yield 6: In the N_2 glovebox, **4a** (19 mg, 0.025 mmol) was dissolved in THF (1.0 mL) at -30°C under N_2 (1 atm). After 1 day at -30°C , the solution was evaporated and dissolved in small amount of DME and crystallized at -30°C . After a few days, microcrystalline precipitates of $[\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-}\eta^2\text{:}\eta^2\text{:}\eta^1\text{-CH=CCH}_3)(\mu_3\text{-}\eta^2\text{:}\eta^2\text{:}\eta^1\text{-N}_2)(\mu\text{-H})]$ (**6**) (11 mg, 0.014 mmol, 56%) were formed as dark brown solid. Single crystals of **6** suitable for X-ray study were obtained from DME solution at -30°C .

Characterization of 6: ^1H NMR (C_6D_6 , rt): δ 9.14 (s, 1H, =CH-), 2.62, 2.41, 2.39, 2.35, 2.18, 2.17, 2.11, 2.02, 1.95, 1.81, 1.48, 1.40, 1.27 (s, $3\text{H}\times 13$, $\text{C}_5\text{Me}_4\text{SiMe}_3$ or Me), 0.57 (s, 9H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 0.38 (s, 9H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 0.20 (s, 9H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), -4.07 (s, 1H, $\mu\text{-H}$). $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , rt): δ 269.6 (s, -MeC=CH-), 217.9 (s, -MeC=CH-), 131.6, 129.8, 129.0, 127.2, 126.4, 124.2, 124.1, 123.5, 122.7, 122.4, 122.0, 121.5, 120.8, 113.2 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 22.5 (s, Me), 16.6, 15.6, 15.4, 15.3, 15.1, 14.9, 12.7, 12.6, 12.1, 12.0, 11.3, 11.2 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 2.7, 2.2, 2.0 (s, $\text{C}_5\text{Me}_4\text{SiMe}_3$). IR (KBr, Nujol mulls, cm^{-1}): 2952 (vs), 2901 (vs), 2853 (vs), 1456 (s), 1375 (s), 1330 (s), 1244 (s), 1128 (m), 1022 (s), 1002 ($\nu_{\text{NN,W}}$), 994 (w), 946 (w), 839 (vs), 754 (s), 686 (s), 631 (s), 579 (m), 531 (s).

Reaction of 4a with $^{15}\text{N}_2$ (1 atm) to yield ^{15}N -labelled 6- ^{15}N and 6'- ^{15}N : J. Young valve NMR sample tube was charged with C_6D_6 (0.4 mL) and complex **4a** (11 mg, 0.014 mmol). The solution was frozen in liquid nitrogen, degassed and $^{15}\text{N}_2$ gas (1 atm) was added. The reaction was kept at room temperature and monitored by $^{15}\text{N}\{^1\text{H}\}$ NMR. After 3 h, the ^{15}N -labelled complex $[\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-}\eta^2\text{:}\eta^2\text{:}\eta^1\text{-CH=CCH}_3)(\mu_3\text{-}$

$\eta^2:\eta^2:\eta^1\text{-}^{15}\text{N}_2)(\mu\text{-H})]$ (**6**- ^{15}N) was produced as the major product together with the formation of minor ^{15}N -labelled complex **6'**- ^{15}N .

Characterization of 6- ^{15}N : $^{15}\text{N}\{^1\text{H}\}$ NMR (C_6D_6 , rt): major δ 216.5 (d, $J_{\text{NN}} = 21.8$ Hz, $^{15}\text{N}\text{-}^{15}\text{N}$), 42.1 (d, $J_{\text{NN}} = 21.8$ Hz, $^{15}\text{N}\text{-}^{15}\text{N}$). IR (KBr, Nujol mulls, cm^{-1}): 2952 (vs), 2917 (vs), 2853 (vs), 1456 (s), 1374 (s), 1329 (s), 1245 (s), 1128 (m), 1022 (s), 994 (w), 971 ($\nu^{15}\text{N}\text{-}^{15}\text{N}$, w), 946 (w), 839 (vs), 755 (s), 687 (s), 631 (s), 569 (m), 523 (s).

Characterization of 6'- ^{15}N : $^{15}\text{N}\{^1\text{H}\}$ NMR (C_6D_6 , rt): δ 210.2 (d, $J_{\text{NN}} = 21.7$ Hz, $^{15}\text{N}\text{-}^{15}\text{N}$), 48.0 (d, $J_{\text{NN}} = 21.7$ Hz, $^{15}\text{N}\text{-}^{15}\text{N}$).

The ^{15}N -labelled complex $[(\text{C}_5\text{Me}_4\text{SiMe}_3\text{Ti})_3(\mu_3\text{-}\eta^2:\eta^2:\eta^1\text{-CH=CCH}_3)(\mu_3\text{-}\eta^2:\eta^2:\eta^1\text{-}^{15}\text{N}_2)(\mu\text{-H})]$ (**6**- ^{15}N) and its minor ^{15}N -labelled complex **6'**- ^{15}N were observed when the reaction of **4a** with $^{15}\text{N}_2$ (1 atm) in C_6D_6 was monitored by $^{15}\text{N}\{^1\text{H}\}$ NMR (Fig. S46). The $^{15}\text{N}\{^1\text{H}\}$ NMR spectrum showed two sets of two doublet signals at δ_{N} 216.5 (d, $J_{\text{NN}} = 21.8$ Hz), 42.1 (d, $J_{\text{NN}} = 21.8$ Hz) as major signals and δ_{N} 210.2 (d, $J_{\text{NN}} = 21.7$ Hz), 48.0 (d, $J_{\text{NN}} = 21.7$ Hz) as minor signals, which were assigned as the reduced $^{15}\text{N}\text{-}^{15}\text{N}$ units in **6**- ^{15}N and its isomer **6'**- ^{15}N . The J_{NN} value and the large difference in chemical shift between two $^{15}\text{N}\{^1\text{H}\}$ NMR signals of **6**- ^{15}N are comparable to those observed in the dinitrogen complex $[(\text{Cp}'\text{Ti})_3(\mu_3\text{-}\eta^1:\eta^2:\eta^2\text{-}^{15}\text{N}_2)(\mu\text{-H})_3]$ (δ_{N} 262.9, 73.1, $J_{\text{NN}} = 21.5$ Hz). Complex **6**- ^{15}N for the IR measurement was prepared from **4a** and $^{15}\text{N}_2$ (1 atm) in THF-d_8 at -30 °C for 2 days. Characterization of the N–N stretching vibration has been achieved by a comparison of the IR spectra of **6** and **6**- ^{15}N ($^{14}\text{N}/^{15}\text{N}$ at $1002/971$ cm^{-1}) (Fig. S50).

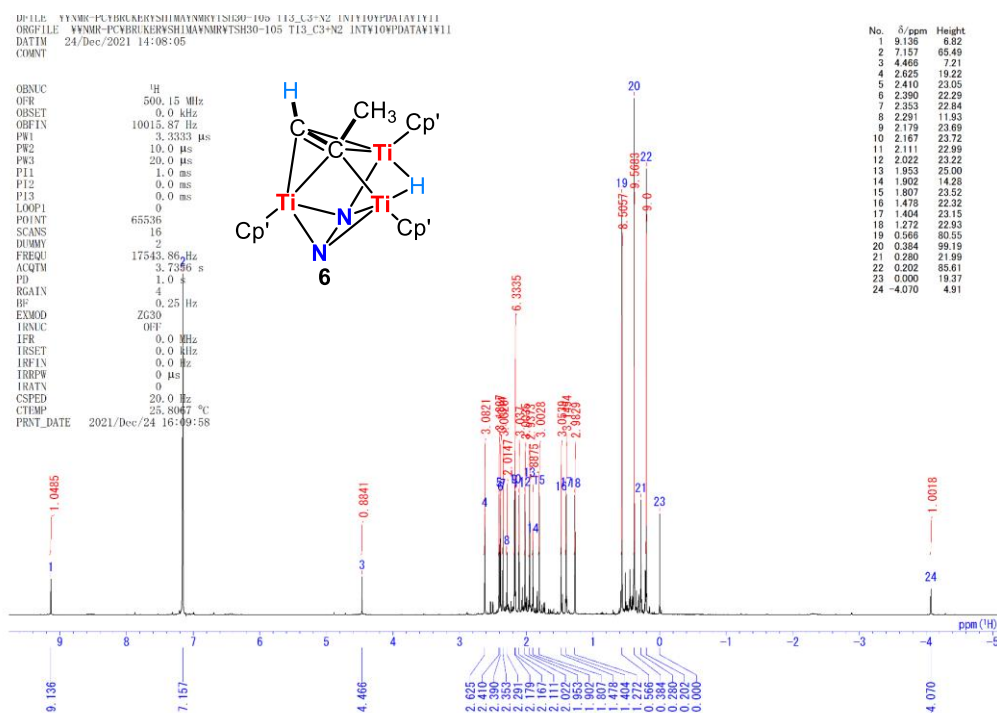


Figure S48. ^1H NMR spectrum of **6** (C_6D_6 , rt).

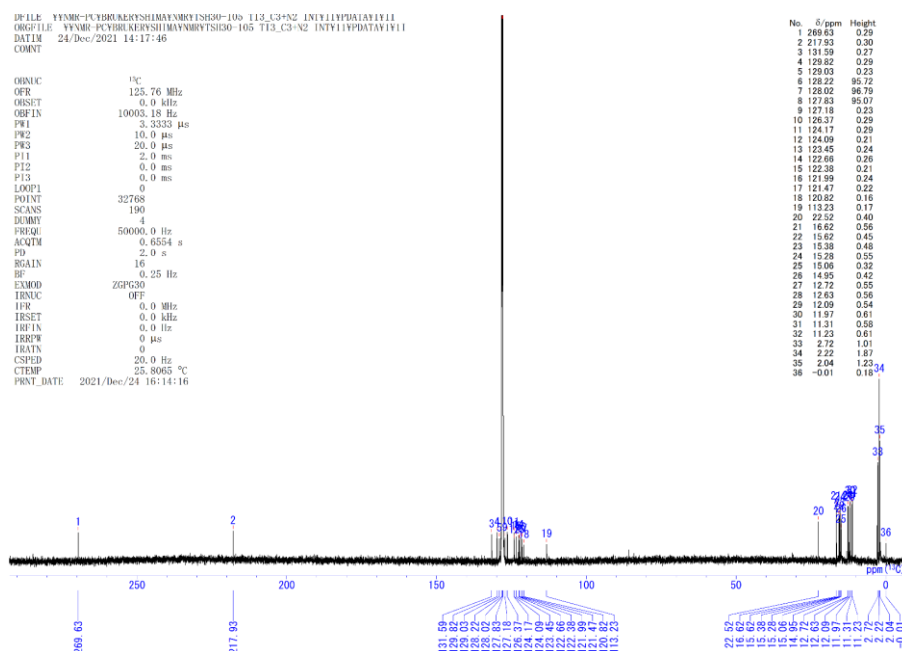


Figure S49. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **6** (C_6D_6 , rt).

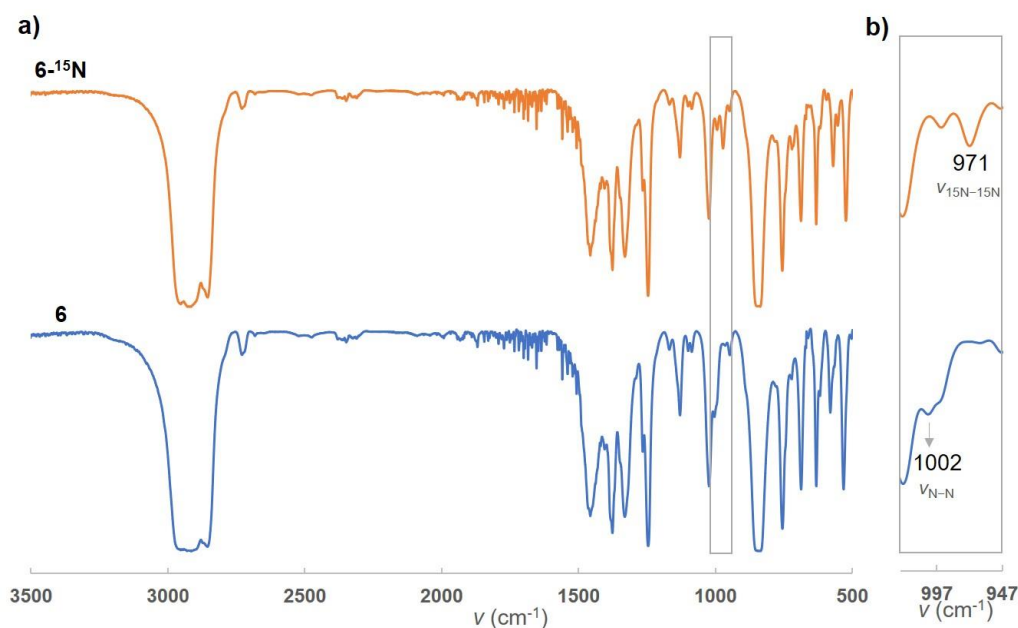


Figure S50. IR spectra of isotopologues of **6**. a). Stacked IR spectra of **6** and $6\text{-}^{15}\text{N}$. b). Stacked partial IR spectra of **6** and $6\text{-}^{15}\text{N}$.

^1H NMR monitoring of the reaction of **4a with N_2 (5 atm):** A 5-mm pressure NMR tube (Wilmad Lab Glass) was charged with **4a** (5.0 mg, 0.0065 mmol) and C_6D_6 (0.40 mL, 9.8 mM) in a glovebox. The solution was degassed under vacuum. High pressure N_2 gas (5 atm) was then introduced to the NMR tube. The sample was monitored at room temperature by ^1H NMR spectroscopy (Fig. S51). After 20 minutes, complex **4a** was disappeared and complex **6** was quantitatively formed. The ^1H NMR spectrum of **6** showed the $\alpha\text{-CH}$ proton and the hydride signals at δ 9.14 (1H) and -4.07 (1H), respectively. After 3 h, the formation of the minor complex **6'** (~20%) was also

observed. Complexes **6** and **6'** were slowly converted to **5** at room temperature for 2 days.

Characterization of 6': ^1H NMR (partially assignment, C_6D_6 , rt): δ 6.69 (s, 1H, =CH-), -2.88 (s, 1H, $\mu\text{-H}$).

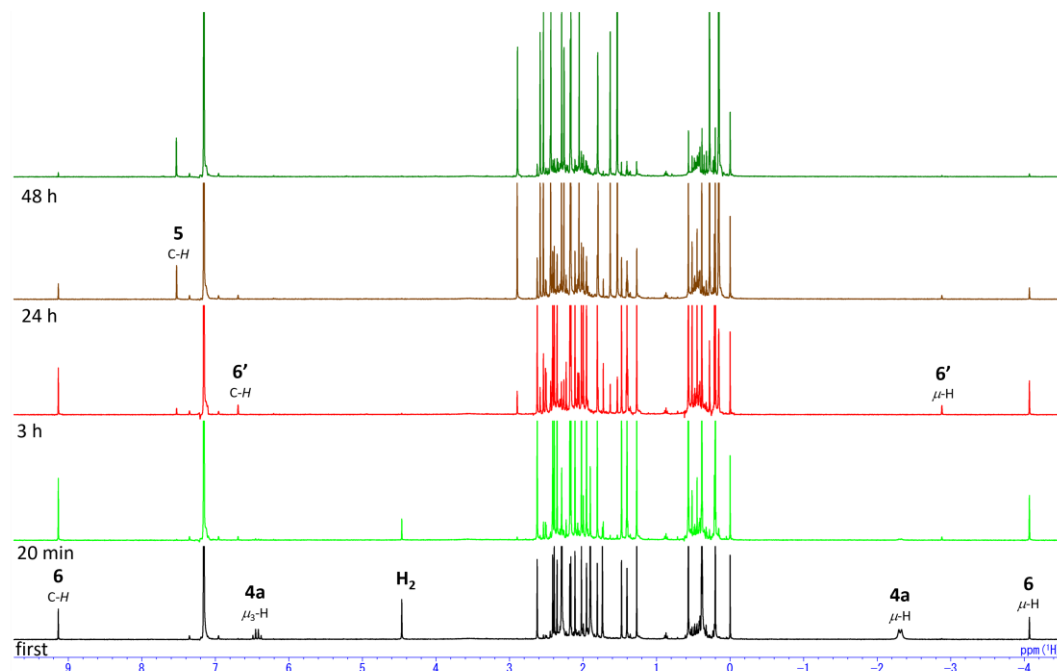


Figure S51. ^1H NMR monitoring of the reaction of **4a** with N_2 (5 atm) in C_6D_6 (rt).

Reaction of 5 with H_2 (4 atm) to yield **8a:** A hexane solution (3.0 mL) of **5** (100 mg, 0.126 mmol) in 10 mL Hiper Glass Cylinder (TAIATSU TECHNO[®]) was filled with 4 atm of H_2 . The solution was kept at room temperature for 1 day with stirring. After the reaction, the solution was evaporated and the residual dark brown powder was crystallized in DME at $-30\text{ }^\circ\text{C}$ to precipitate $[\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-N})(\mu\text{-NCH}(\text{CH}_3)_2)(\mu\text{-H})_2]$ (**8a**) (83 mg, 0.104 mmol, 83%) as a black crystalline solid. Single crystals of **8a** suitable for X-ray study were obtained from DME/benzene solution at $-30\text{ }^\circ\text{C}$.

Reaction of 4a with N_2 (5 atm) and H_2 (4 atm) to yield **8a:** A hexane solution (2.0 mL) of **4a** (51 mg, 0.067 mmol) in 10 mL Hiper Glass Cylinder (TAIATSU TECHNO[®]) was filled with 5 atm of N_2 . The solution was stirred at room temperature for 2 days. After the reaction, N_2 was released and H_2 (4 atm) was filled instead. The solution was kept at room temperature for 1 day with stirring. After the reaction, the solution was evaporated under reduced pressure and the residual dark brown powder was crystallized in hexane/benzene (10/1) at $-30\text{ }^\circ\text{C}$ to precipitate the crystalline solid $[\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-N})(\mu\text{-NCH}(\text{CH}_3)_2)(\mu\text{-H})_2]$ (**8a**) (30 mg, 0.038 mmol). The solution part was evaporated under reduced pressure and the residual dark brown powder was crystallized in DME at $-30\text{ }^\circ\text{C}$ to precipitate the microcrystalline solid **8a** (13 mg, 0.013 mmol). Overall yield of **8a** is 72%.

Characterization of **8a:** ^1H NMR (C_6D_6 , rt): δ 16.63 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 9.25 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 7.91 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 5.25 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 3.98 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 3.49 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 2.72 (s, 6H, $-\text{CHMe}_2$), 1.16 (s, 9H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 0.79 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), -2.56 (s, 1H, $-\text{CHMe}_2$). Anal. calcd. for $\text{C}_{39}\text{H}_{72}\text{N}_2\text{Si}_3\text{Ti}_3$: C, 58.78; H, 9.11; N, 3.52. Found: C, 58.33; H, 9.14; N, 3.27. FD-MS: $m/z = 796.4$ ($[\mathbf{8a}]^+$). $\mu_{\text{eff}}(298\text{K}) = 1.5 \mu_{\text{B}}$.

In agreement of the presence of the weak Ti(III)–Ti(III) bonding interactions (magnetic susceptibility $\mu_{\text{eff}} = 1.5 \mu_{\text{B}}$) (ref. 6), complex **8a** exhibited paramagnetic behavior and showed poorly-resolved signals in the ^1H NMR spectrum (Fig. S52). The field desorption mass (FD-MS) spectrum of **8a** showed the signal of $[\mathbf{8a}]^+$ at m/z 796.4, in agreement with its formula assignment (Fig. S53).

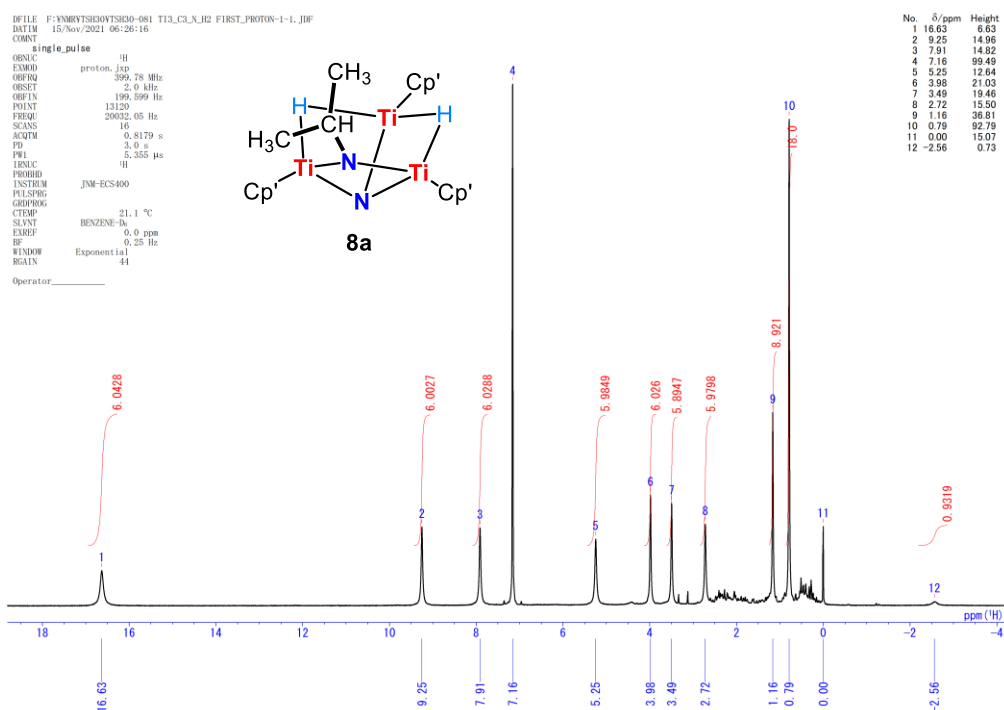


Figure S52. ^1H NMR spectrum of **8a** (C_6D_6 , rt).

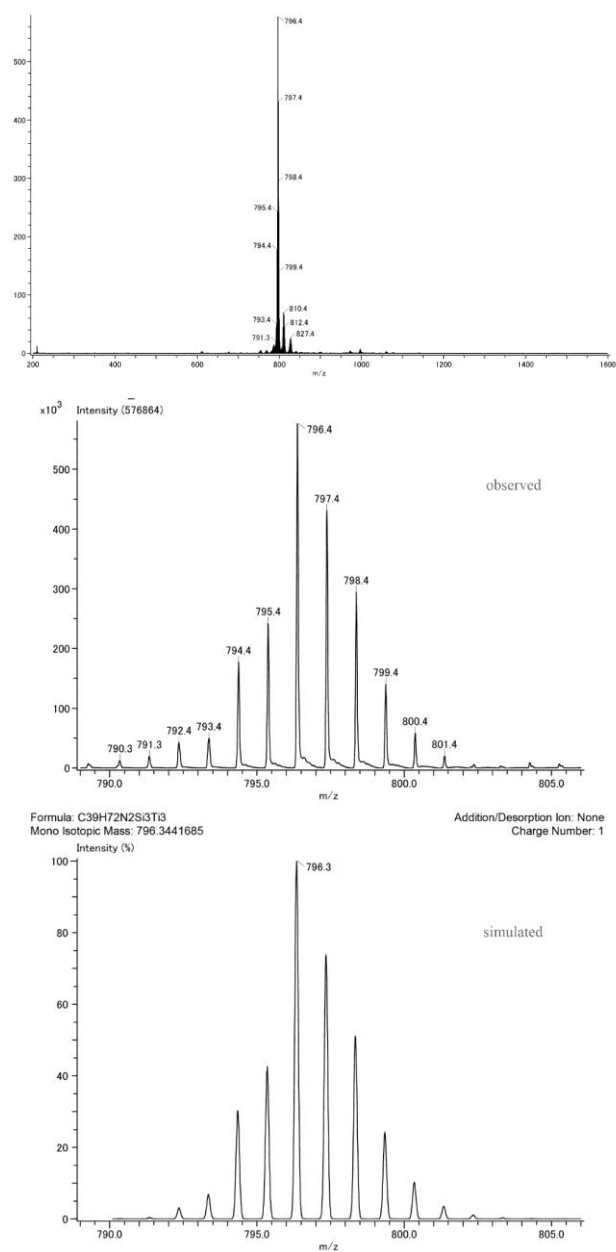


Figure S53. FD-MS spectra of **8a**.

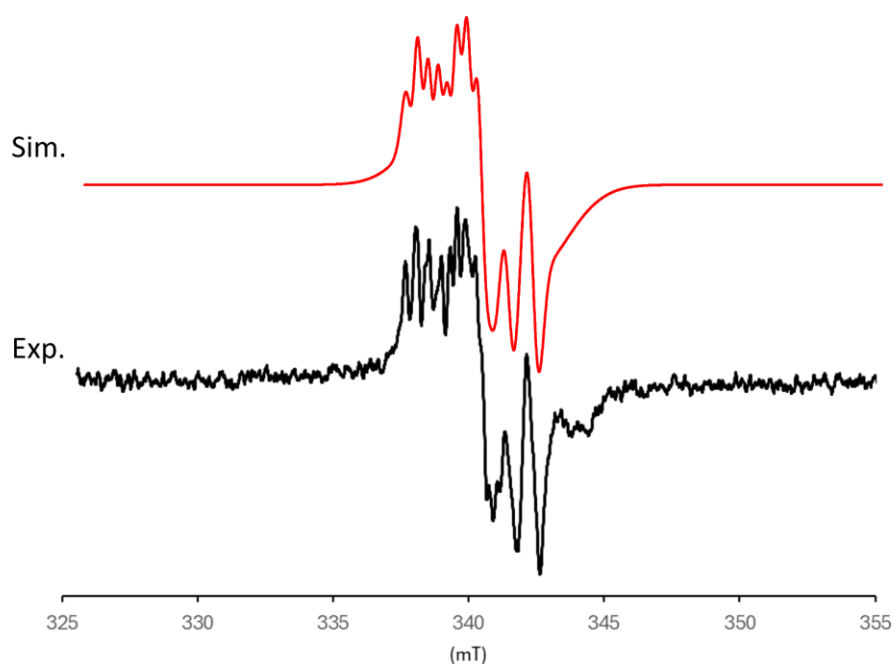
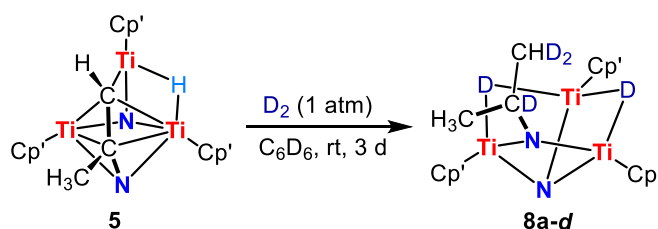


Figure S54. Experimental (black) and simulated (red) X-band EPR spectra of complex **8a** recorded in toluene solution at 298 K. EPR spectrum of **8a** was simulated by Easyspin. Major signal was derived from Ti(III) atoms ($g = 1.981$). Two nitrogen, two hydride, and the hydrogen nuclei on *ipso*-*i*Pr group have hyperfine interactions with unpaired electron. The hyperfine couplings from nitrogen and hydrogen atoms [$A_{^{14}\text{N}}$, $A_{^1\text{H}}$] are [25.84, 0] (for $\mu_3\text{-}^{14}\text{N}$), [12.52, 6.72] (for $\mu\text{-}^{14}\text{N}^i\text{Pr}$), [19.71, 10.60] (for $\mu\text{-}^1\text{H}$), and [19.73, 10.88] (for *ipso*-*i*Pr) (MHz), respectively.

Reaction of 5 with D₂ (1 atm) to yield deuterium-labelled 8a-d:



A J. Young valve NMR sample tube was charged with 0.4 mL of C₆D₆ and complex **5** (8 mg). The solution was degassed and 1 atm of D₂ gas was added. The solution was kept at room temperature for 3 days and the ¹H NMR monitoring showed the formation of the deuterated complex [$\{(\text{C}_5\text{Me}_4\text{SiMe}_3\text{Ti})_3(\mu_3\text{-N})(\mu\text{-NCD}(\text{CH}_3)(\text{CHD}_2))(\mu\text{-D})_2\}$] (**8a-d**).

Characterization of 8a-d: ¹H NMR (C₆D₆, rt): δ 2.69 (s, 4H, (CH₃)(CHD₂)). ²H NMR (C₆H₆, rt): δ 2.7 (brs, CD(CH₃)(CHD₂)), -1.4 (brs, CD(CH₃)(CHD₂)).

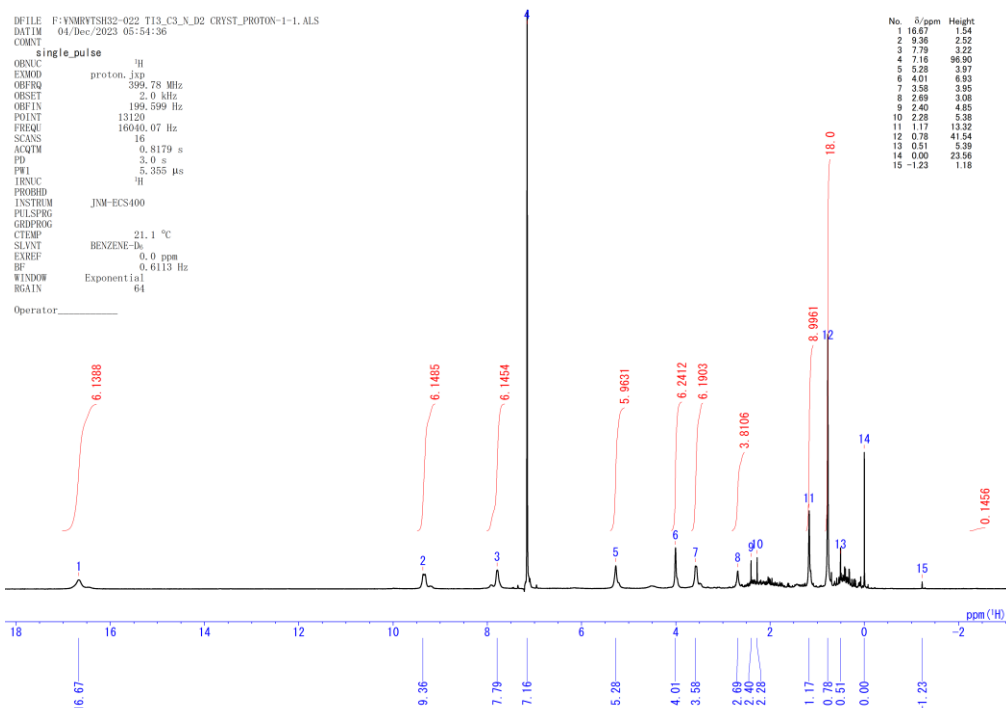


Figure S55. ¹H NMR spectrum of **8a-d** (C₆D₆, rt).

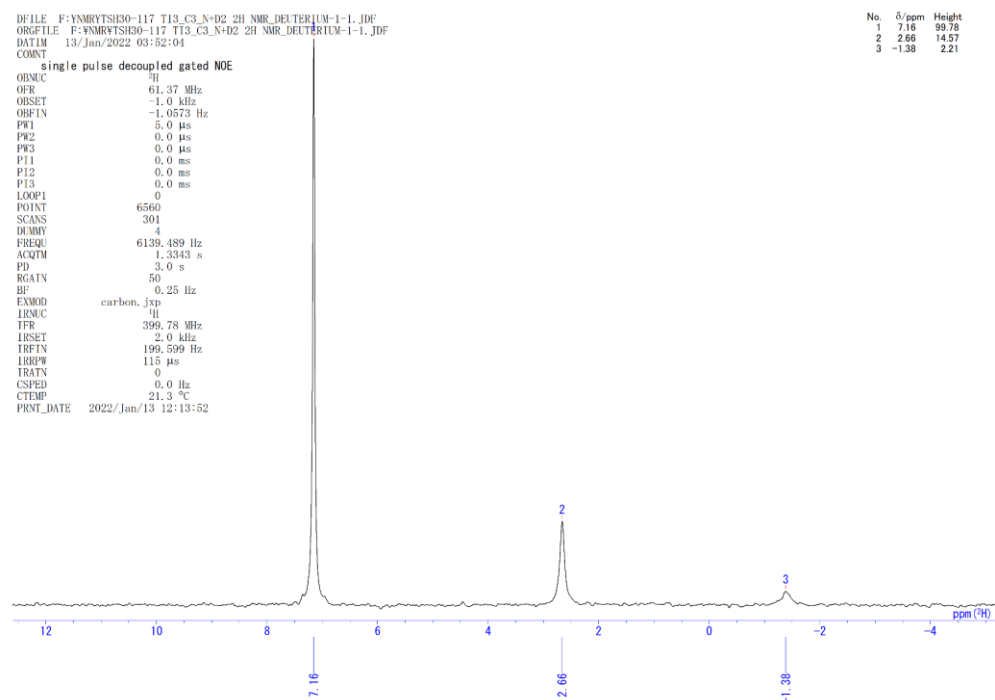


Figure S56. ²H NMR spectrum of **8a-d** (C₆H₆, rt).

Reaction of 4b with N₂ (5 atm) and H₂ (4 atm) to yield 8b: A hexane solution (2.0 mL) of **4b** (81 mg, 0.10 mmol) in 10 mL Hiper Glass Cylinder (TAIATSU TECHNO[®]) was filled with 5 atm of N₂. The solution was stirred at room temperature for 2 days. After the reaction, N₂ was released and H₂ (4 atm) was filled instead. The solution was kept at room temperature for 1 day with stirring. After the reaction, the solution was evaporated and the residual dark brown powder was crystallized in DME (~0.5 mL) at –30 °C to precipitate the crystalline solid [(Cp'Ti)₃(μ₃-N)(μ-NH)(μ-H)₂] (**2**) (5.0 mg, 0.0066 mmol, 7%). The solution part was concentrated and recrystallized at –30 °C to give the complex [{(C₅Me₄SiMe₃)Ti}₃(μ₃-N)(μ-NCH(CH₃)(CH₂CH₃))(μ-H)₂] (**8b**) (50 mg, 0.062 mmol, 62%) as a dark green solid. (The formation of **2** could proceed through N–C bond cleavage of the organic unit in the alkenylimide intermediates such as **5** or **8b** followed by hydrogenolysis to release the corresponding hydrocarbon species.)

Characterization of 8b: ¹H NMR (C₆D₆, rt): δ 16.17 (s, 3H, C₅Me₄SiMe₃), 15.81 (s, 3H, C₅Me₄SiMe₃), 9.10 (s, 3H, C₅Me₄SiMe₃), 8.91 (s, 3H, C₅Me₄SiMe₃), 8.29 (s, 3H, C₅Me₄SiMe₃), 6.90 (s, 3H, C₅Me₄SiMe₃), 5.01 (s, 3H, C₅Me₄SiMe₃), 4.88 (s, 3H, C₅Me₄SiMe₃), 3.92 (s, 1H, -CHCH₂CH₃), 3.69 (s, 3H, C₅Me₄SiMe₃), 3.65 (s, 3H, C₅Me₄SiMe₃), 3.61 (s, 3H, C₅Me₄SiMe₃), 3.07 (s, 3H, -CHCH₃), 2.75 (s, 3H, C₅Me₄SiMe₃), 2.21 (brs, 1H, -CHCH₂CH₃), 1.34 (s, 3H, -CHCH₂CH₃), 0.94 (s, 9H, C₅Me₄SiMe₃), 0.73 (s, 9H, C₅Me₄SiMe₃), 0.66 (s, 9H, C₅Me₄SiMe₃), –1.27 (s, 1H, -CHCH₃). ¹H-¹H COSY (C₆D₆, rt): δ_H 3.92-2.21, 1.34; δ_H 2.21-3.92, 1.34; δ_H 1.34-3.92, 2.21. Anal. calcd. for C₄₀H₇₄N₂Si₃Ti₃: C, 59.25; H, 9.20; N, 3.45. Found: C, 59.23; H, 8.99; N, 3.55.

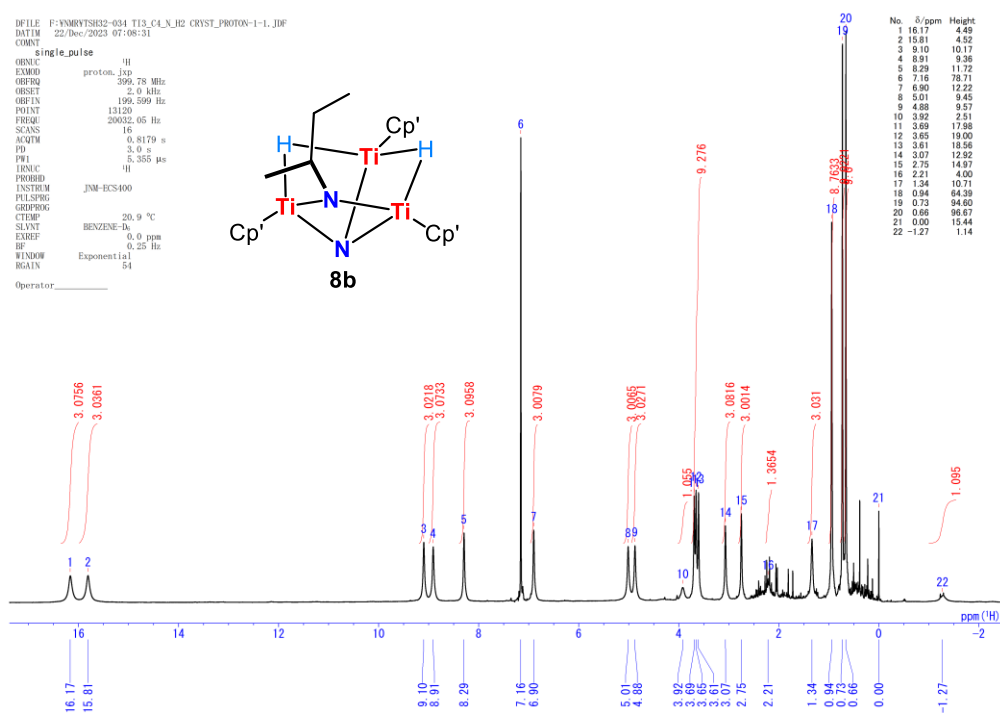


Figure S57. ¹H NMR spectrum of **8b** (C₆D₆, rt).

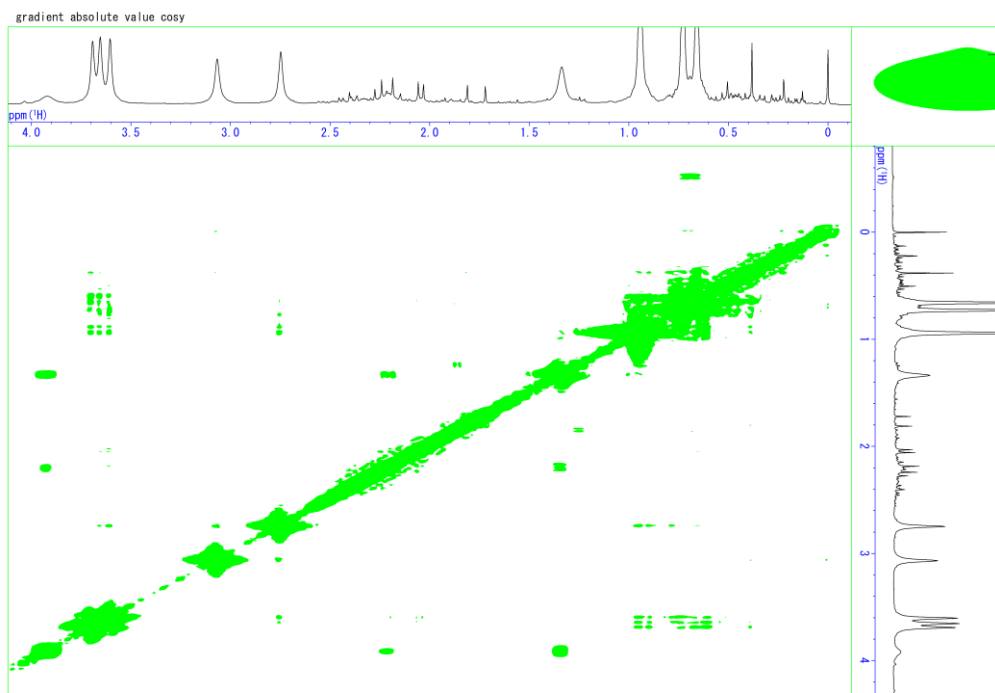


Figure S58. ^1H - ^1H COSY spectrum of **8b** (C_6D_6 , rt).

Reaction of 4c with N_2 (5 atm) and H_2 (4 atm) to yield 8c: A hexane solution (2.0 mL) of **4c** (62 mg, 0.078 mmol) in 10 mL Hiper Glass Cylinder (TAIATSU TECHNO[®]) was filled with 5 atm of N_2 . The solution was stirred at room temperature for 2 days. After the reaction, N_2 was released and H_2 (4 atm) was filled instead. The solution was kept at room temperature for 1 day with stirring. After the reaction, the solution was evaporated and the residual dark brown powder was crystallized in DME (~ 0.3 mL) at -30 $^\circ\text{C}$ to precipitate the crystalline solid $[(\text{Cp}'\text{Ti})_3(\mu_3\text{-N})(\mu\text{-NH})(\mu\text{-H})_2]$ (**2**) (2.0 mg, 0.0027 mmol, 3%). The solution part was evaporated under reduced pressure to give the complex $[\{(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{Ti}\}_3(\mu_3\text{-N})(\mu\text{-NCH}(\text{CH}_3)(\text{CH}_2\text{CH}_2\text{CH}_3))(\mu\text{-H})_2]$ (**8c**) (54 mg, 0.065 mmol, 83%) as a dark green solid (no crystals were obtained).

Characterization of 8c: ^1H NMR (C_6D_6 , rt): δ 16.55 (s, 3H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 15.91 (s, 3H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 9.16 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 8.41 (s, 3H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 6.88 (s, 3H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 5.19 (s, 3H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 4.81 (s, 3H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 3.80 (s, 4H, $\text{C}_5\text{Me}_4\text{SiMe}_3 + \text{-CH}_2\text{-}$), 3.65 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 3.17 (s, 3H, $\text{CH}_3\text{-CHN-}$), 2.66 (s, 3H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 2.23 (brs, 1H, $\text{-CH}_2\text{-}$), 1.63 (brs, 1H, $\text{-CH}_2\text{-}$), 1.52 (brs, 1H, $\text{-CH}_2\text{-}$), 1.13 (s, 3H, $\text{-CH}_2\text{CH}_3$), 0.94 (s, 9H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 0.72 (s, 9H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 0.64 (s, 9H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), -0.79 (s, 1H, -CHCH_3). ^1H - ^1H COSY (C_6D_6 , rt): δ_{H} 3.80-2.23, 1.52; δ_{H} 2.23-3.80, 1.63; δ_{H} 1.63-2.23, 1.13; δ_{H} 1.52-3.80, 1.13; δ_{H} 1.13-1.63, 1.52; δ_{H} -0.79 -3.17. Anal. calcd. for $\text{C}_{41}\text{H}_{76}\text{N}_2\text{Si}_3\text{Ti}_3$: C, 59.70; H, 9.29; N, 3.40. Found: C, 59.13; H, 8.98; N, 3.71.

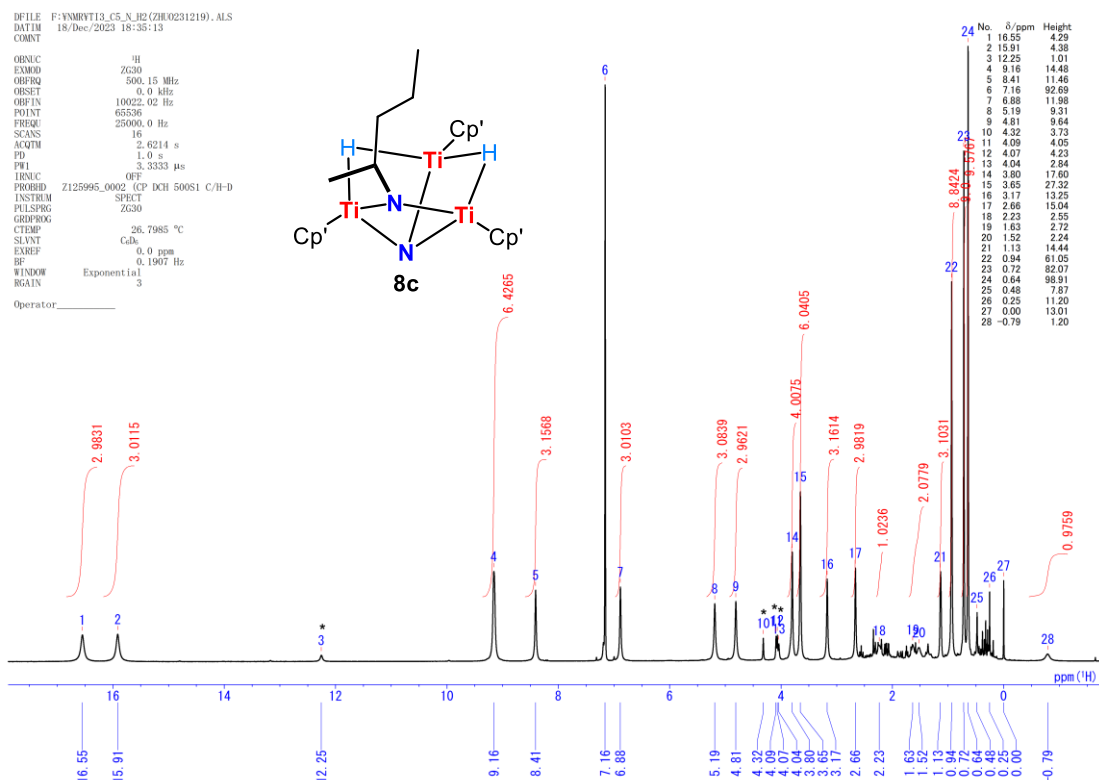


Figure S59. ¹H NMR spectrum of **8c** (C₆D₆, rt). *Inseparable signals of complex **2** were observed.

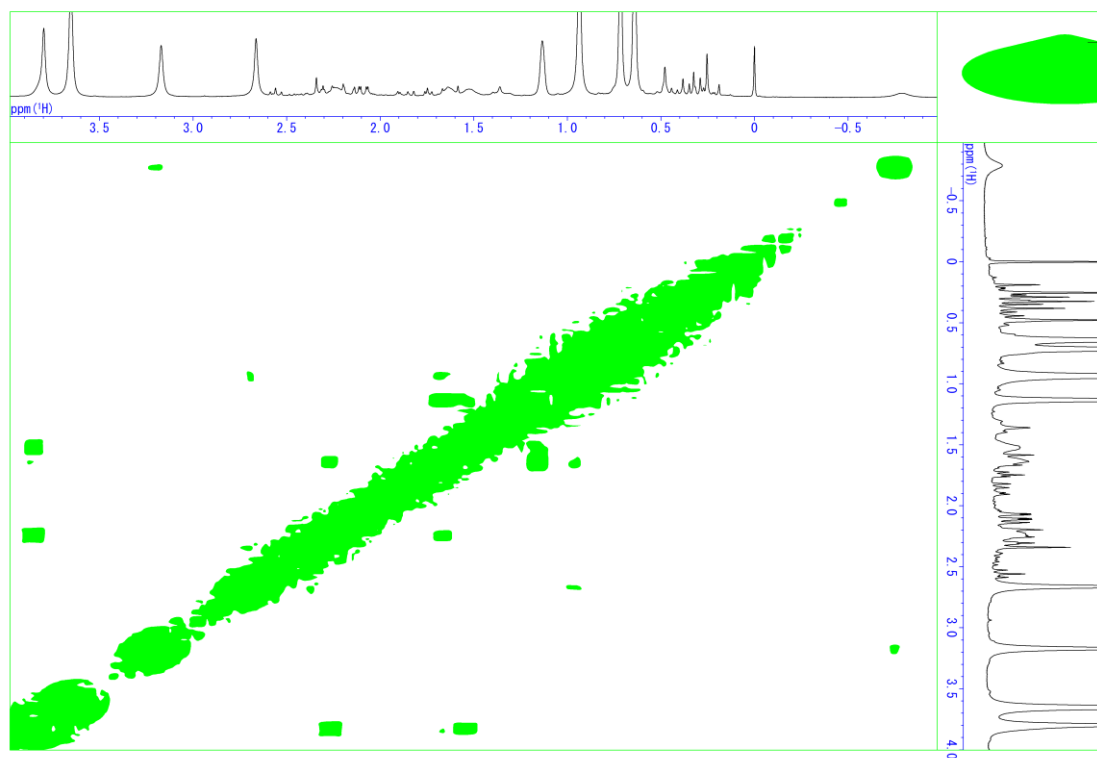


Figure S60. ¹H-¹H COSY spectrum of **8c** (C₆D₆, rt).

Reaction of 4d with N₂ (5 atm) and H₂ (4 atm) to yield 8d: A hexane solution (2.0 mL) of **4d** (58 mg, 0.071 mmol) in 10 mL Hiper Glass Cylinder (TAIATSU TECHNO[®]) was filled with 5 atm of N₂. The solution was stirred at room temperature for 2 days. After the reaction, N₂ was released and H₂ (4 atm) was filled instead. The solution was kept at room temperature for 1 day with stirring. After the reaction, the solution was evaporated and the residual dark brown powder was crystallized in DME at –30 °C to precipitate the crystalline solid [(Cp'Ti)₃(μ₃-N)(μ-NH)(μ-H)₂] (**2**) (5.0 mg, 0.0066 mmol, 9%). The solution part was evaporated under reduced pressure to give the complex [(C₅Me₄SiMe₃)Ti]₃(μ₃-N)(μ-NCH(CH₃)(CH₂CH₂CH₂CH₃))(μ-H)₂] (**8d**) (50 mg, 0.060 mmol, 84%) as a dark green solid (no crystals were obtained).

Characterization of 8d: ¹H NMR (C₆D₆, rt): δ 16.37 (s, 3H, C₅Me₄SiMe₃), 15.95 (s, 3H, C₅Me₄SiMe₃), 9.16 (s, 3H, C₅Me₄SiMe₃), 8.95 (s, 3H, C₅Me₄SiMe₃), 8.45 (s, 3H, C₅Me₄SiMe₃), 6.95 (s, 3H, C₅Me₄SiMe₃), 5.13 (s, 3H, C₅Me₄SiMe₃), 4.96 (s, 3H, C₅Me₄SiMe₃), 3.75 (s, 4H, C₅Me₄SiMe₃ + -CH₂-), 3.68 (s, 3H, C₅Me₄SiMe₃), 3.66 (s, 3H, C₅Me₄SiMe₃), 3.08 (s, 3H, CH₃-CHN-), 2.78 (s, 3H, C₅Me₄SiMe₃), 2.51 (brs, 1H, -CH₂-), 1.92 (brs, 2H, -CH₂-), 1.52 (brs, 1H, -CH₂-), 1.45 (brs, 1H, -CH₂-), 0.98 (s, 9H, C₅Me₄SiMe₃), 0.89 (t, J = 6.7 Hz, 3H, -CH₂CH₃), 0.74 (s, 9H, C₅Me₄SiMe₃), 0.67 (s, 9H, C₅Me₄SiMe₃), –0.79 (s, 1H, -CHMe). Anal. calcd. for C₄₂H₇₈N₂Si₃Ti₃: C, 60.13; H, 9.37; N, 3.34. Found: C, 59.92; H, 8.89; N, 3.67.

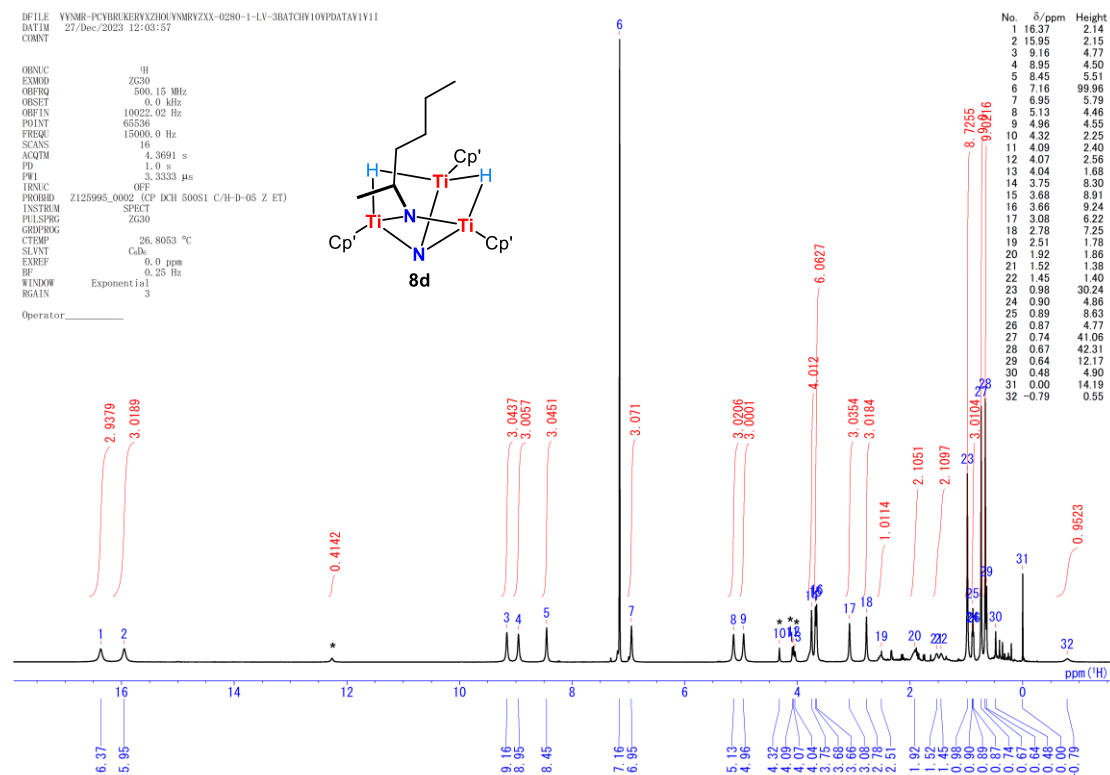


Figure S61. ¹H NMR spectrum of **8d** (C₆D₆, rt). *Inseparable signals of complex **2** were observed.

Reaction of 4e with N₂ (5 atm) and H₂ (4 atm) to yield 8e: A hexane solution (2.0 mL) of **4e** (60 mg, 0.072 mmol) in 10 mL Hiper Glass Cylinder (TAIATSU TECHNO[®]) was filled with 5 atm of N₂. The solution was stirred at 40 °C for 2 days. After the reaction, N₂ was released and H₂ (4 atm) was filled instead. The solution was kept at room temperature for 1 day with stirring. After the reaction, the solution was evaporated and the residual dark brown powder was crystallized in hexane at –30 °C to precipitate the crystalline solid [(Cp'Ti)₃(μ₃-N)(μ-NH)(μ-H)₂] (**2**) (5 mg, 0.0066 mmol, 9%). The solution part was evaporated under reduced pressure to give the complex [{(C₅Me₄SiMe₃)Ti}₃(μ₃-N)(μ-NCH(CH₃)Ph)(μ-H)₂] (**8e**) (45 mg, 0.052 mmol, 72%) as a dark brown solid (no crystals were obtained).

Characterization of 8e: ¹H NMR (C₆D₆, rt): δ 14.64 (s, 3H, C₅Me₄SiMe₃), 13.18 (s, 3H, C₅Me₄SiMe₃), 10.61 (s, 3H, C₅Me₄SiMe₃), 7.65 (s, 3H, C₅Me₄SiMe₃), 7.54 (t, J_{HH} = 7.2 Hz, 1H, Ph), 6.85 (s, 2H, Ph), 6.72 (s, 3H, C₅Me₄SiMe₃), 6.22 (s, 2H, Ph), 5.62 (s, 3H, C₅Me₄SiMe₃), 4.45 (s, 6H, C₅Me₄SiMe₃), 3.88 (s, 3H, C₅Me₄SiMe₃), 3.37 (s, 3H, C₅Me₄SiMe₃), 3.35 (s, 3H, C₅Me₄SiMe₃ or -CH₃), 3.17 (s, 3H, C₅Me₄SiMe₃ or -CH₃), 2.27 (s, 3H, C₅Me₄SiMe₃), 0.75 (s, 9H, C₅Me₄SiMe₃), 0.60 (s, 9H, C₅Me₄SiMe₃), 0.41 (s, 9H, C₅Me₄SiMe₃). Anal. calcd. for C₄₄H₇₄N₂Si₃Ti₃: C, 61.53; H, 8.68; N, 3.26. Found: C, 61.25; H, 8.56; N, 3.57.

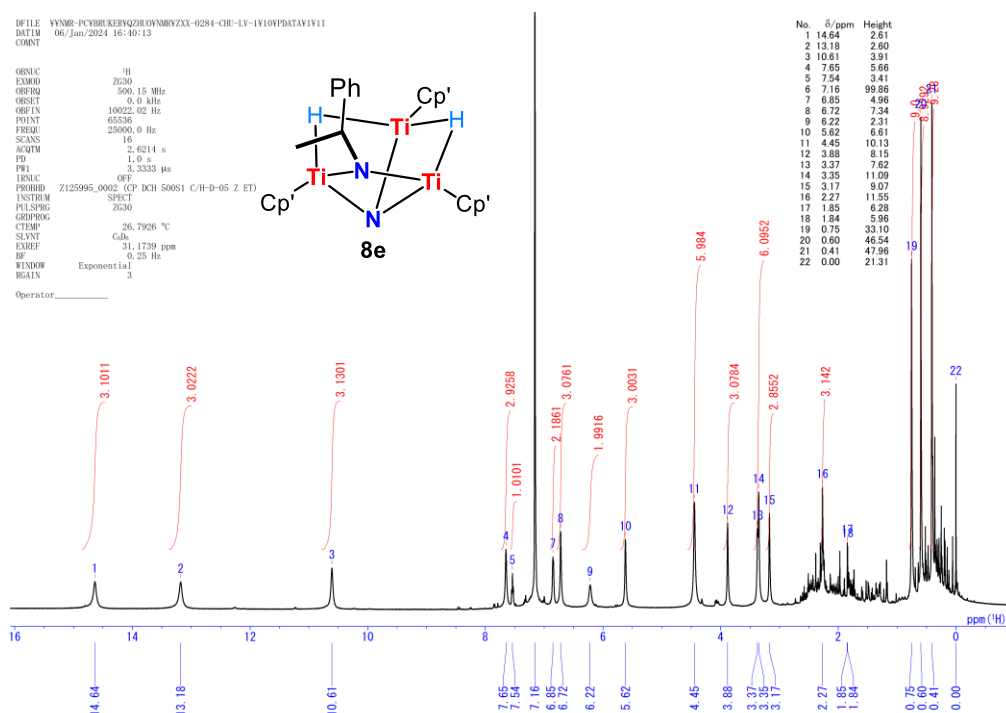


Figure S62. ¹H NMR spectrum of **8e** (C₆D₆, rt).

Reaction of 4f with N₂ (5 atm) and H₂ (10 atm) to yield 8f: A hexane solution (2.0 mL) of **4f** (63 mg, 0.077 mmol) in 10 mL Hiper Glass Cylinder (TAIATSU TECHNO[®]) was filled with 5 atm of N₂. The solution was stirred at room temperature for 1 day. After the reaction, N₂ was released and H₂ (10 atm) was filled at –20 °C. The solution was kept at –20 °C for 19 h with stirring. After the reaction, the solution was evaporated and the residual dark brown powder was crystallized in hexane at –30 °C to precipitate the crystalline solid [(Cp'Ti)₃(μ₃-N)(μ-NH)(μ-H)₂] (**2**) (4 mg, 0.0053 mmol, 7%). The solution part was evaporated under reduced pressure to give the complex [{(C₅Me₄SiMe₃)Ti]₃(μ₃-N)(μ-NCH(CH₃)C₅H₉)(μ-H)₂] (**8f**) (55 mg, 0.065 mmol, 84%) as a dark brown solid (no crystals were obtained).

Characterization of 8f: ¹H NMR (C₆D₆, rt): δ 15.32 (s, 3H, C₅Me₄SiMe₃), 14.14 (s, 3H, C₅Me₄SiMe₃), 9.41 (s, 3H, C₅Me₄SiMe₃), 8.28 (s, 3H, C₅Me₄SiMe₃), 6.91 (s, 3H, C₅Me₄SiMe₃), 5.83 (s, 3H, C₅Me₄SiMe₃), 4.72 (s, 3H, C₅Me₄SiMe₃), 3.96 (s, 3H, C₅Me₄SiMe₃), 3.87 (s, 3H, C₅Me₄SiMe₃), 3.28 (s, 6H, C₅Me₄SiMe₃+ -NCHCH₃), 2.85 (s, 3H, C₅Me₄SiMe₃), 2.38 (brs, 2H, -C₅H₉), 1.94 (brs, 5H, C₅Me₄SiMe₃+ -C₅H₉), 1.81 (brs, 1H, -C₅H₉), 1.51 (brs, 2H, -C₅H₉), 0.99 (brs, 1H, -C₅H₉), 0.60 (s, 9H, C₅Me₄SiMe₃), 0.58 (s, 9H, C₅Me₄SiMe₃), 0.52 (s, 9H, C₅Me₄SiMe₃), 0.30 (brs, 1H, -NCHCH₃), –0.07 (brs, 1H, -C₅H₉). ¹H-¹H COSY (C₆D₆, rt, partially): δ_H 3.28-0.30; δ_H –0.07-2.38, 1.94, 1.51, 0.99. Anal. calcd. for C₄₃H₇₈N₂Si₃Ti₃: C, 60.69; H, 9.24; N, 3.29. Found: C, 59.78; H, 9.31; N, 3.06.

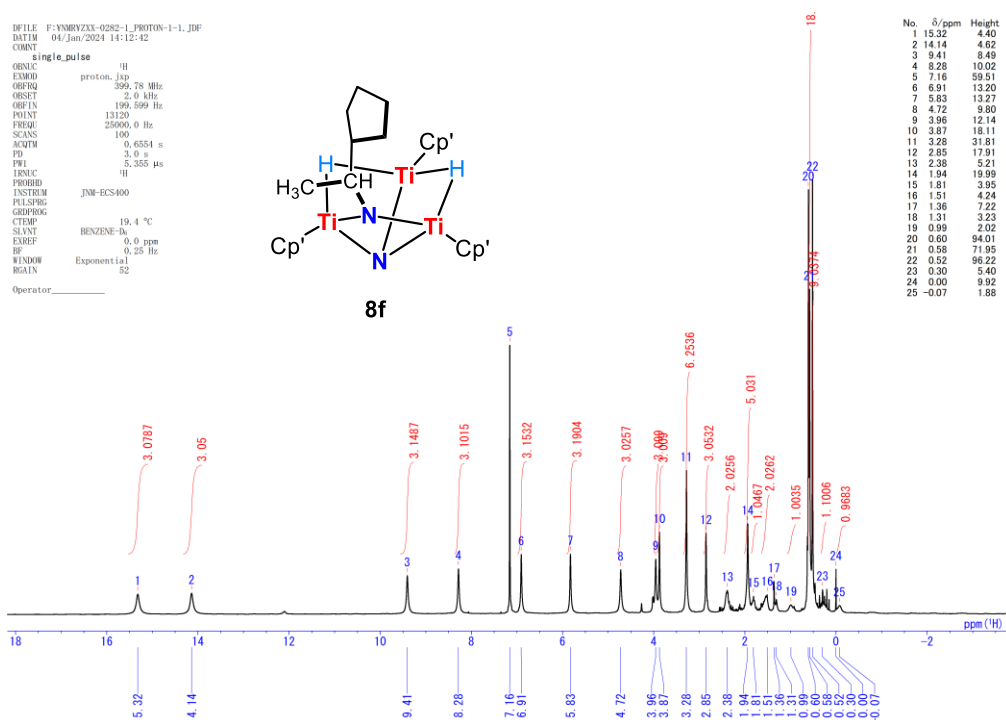


Figure S63. ¹H NMR spectrum of **8f** (C₆D₆, rt).

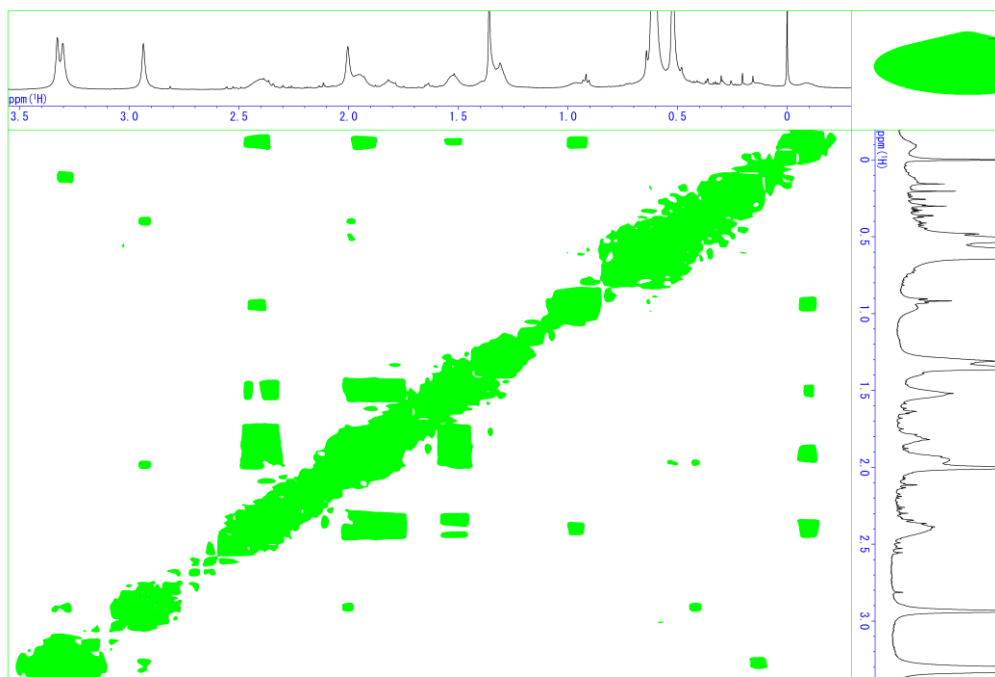


Figure S64. ^1H - ^1H COSY spectrum of **8f** (C_6D_6 , rt).

Reaction of **4g with N_2 (1 atm) and H_2 (1 atm) to yield **8g**:** A C_6D_6 solution (0.5 mL) of **4g** (38 mg, 0.047 mmol) in J. Young NMR tube was filled with 1 atm of N_2 . The solution was stirred at 40°C for 2 days. After the reaction, N_2 was removed and H_2 (1 atm) was filled instead. The solution was kept at 40°C for 1 day. After the reaction, the ^1H NMR showed that the complex **8g** was quantitatively formed. The solution part was evaporated under reduced pressure to give the complex **8g** (40 mg, 0.047 mmol, 100%) as a dark brown solid. Many trials for crystallization of **8g** were failed.

Characterization of **8g:** ^1H NMR (C_6D_6 , rt): δ 17.00 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 9.19 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 8.11 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 5.45 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 4.02 (s, 6H of $\text{C}_5\text{Me}_4\text{SiMe}_3$ and 2H of $-\text{C}_6\text{H}_{11}$), 3.44 (s, 6H of $\text{C}_5\text{Me}_4\text{SiMe}_3$ and 2H of $-\text{C}_6\text{H}_{11}$), 2.82 (brs, 2H, $-\text{C}_6\text{H}_{11}$), 2.31 (m, 1H, $-\text{C}_6\text{H}_{11}$), 2.12 (m, 2H, $-\text{C}_6\text{H}_{11}$), 1.40 (m, 1H, $-\text{C}_6\text{H}_{11}$), 1.19 (s, 9H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), 0.82 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_3$), -1.00 (brs, 1H, $-\text{C}_6\text{H}_{11}$). Anal. calcd. for $\text{C}_{42}\text{H}_{76}\text{N}_2\text{Si}_3\text{Ti}_3$: C, 60.27; H, 9.15; N, 3.35. Found: C, 60.58; H, 9.29; N, 2.81.

Preparation of **8g':** The $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$ -ligated complex [$\{(\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu})\text{Ti}\}_3(\mu_3\text{-N})(\mu\text{-NC}_6\text{H}_{11})(\mu\text{-H})_2$] (**8g'**) was obtained by the reaction of [$\{(\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu})\text{Ti}\}_3(\mu_3\text{-}\eta^2\text{:}\eta^2\text{:}\eta^2\text{-C}_6\text{H}_7)(\mu\text{-H})_3(\mu_3\text{-H})$] (**4g'**) with N_2 , followed by reaction with H_2 , providing crystals suitable for an X-ray diffraction study (toluene, -30°C).

Characterization of **8g':** ^1H NMR (C_6D_6 , rt): δ 18.66 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 12.09 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 11.59 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 4.83 (s, 2H, $-\text{C}_6\text{H}_{11}$), 3.73 (s, 12H of $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$ and 1H of $-\text{C}_6\text{H}_{11}$), 3.58 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 3.39 (s, 2H, $-\text{C}_6\text{H}_{11}$), 3.02 (s, 2H, $-\text{C}_6\text{H}_{11}$), 2.51 (m, 1H, $-\text{C}_6\text{H}_{11}$), 2.21 (m, 2H, $-\text{C}_6\text{H}_{11}$), 1.81 (s, 9H,

$\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 1.44 (s, 18H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 0.76 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 0.32 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), 0.28 (s, 6H, $\text{C}_5\text{Me}_4\text{SiMe}_2^t\text{Bu}$), -2.82 (brs, 1H, $-\text{C}_6\text{H}_{11}$).

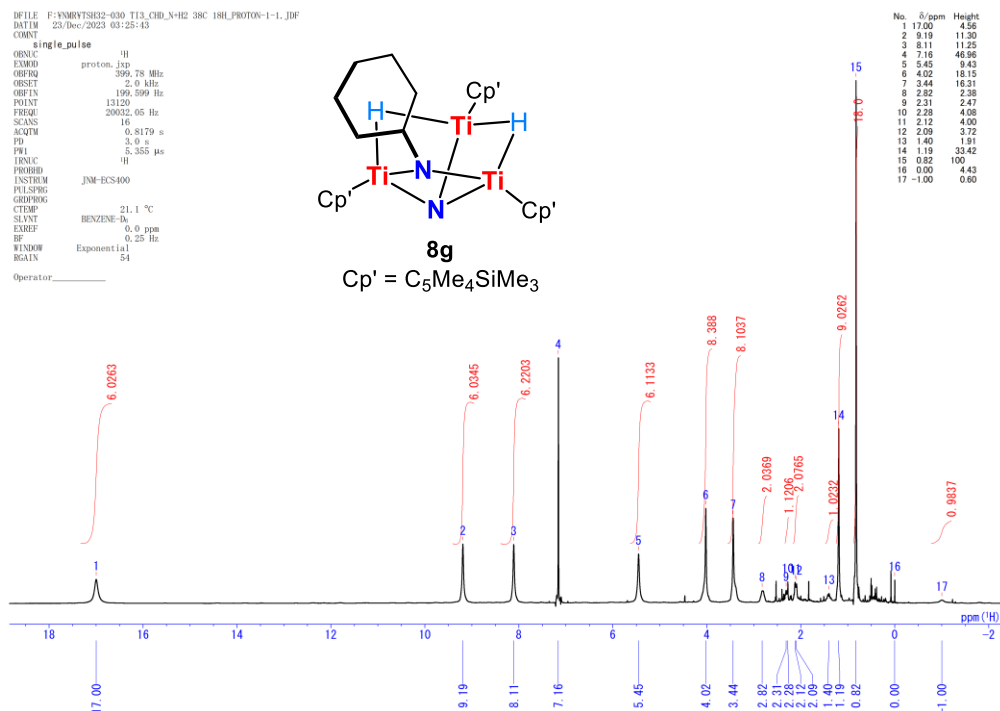


Figure S65. ^1H NMR spectrum of **8g** (C_6D_6 , rt).

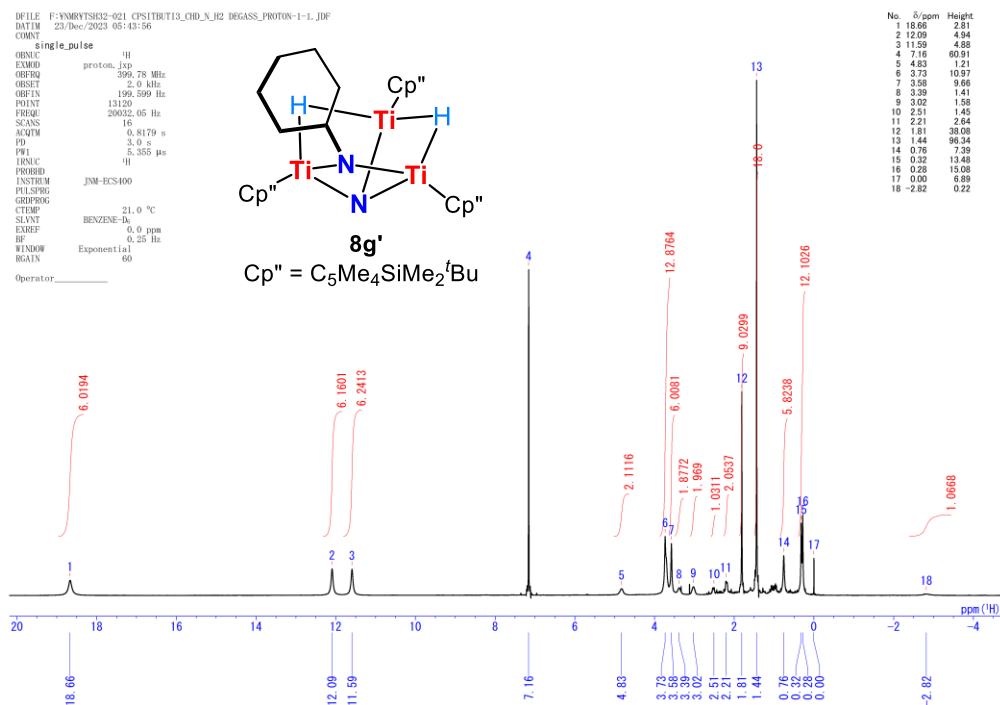


Figure S66. ^1H NMR spectrum of **8g'** (C_6D_6 , rt).

Hydrolysis of 3 with H₂O: Degassed H₂O (5.0 M in THF, 0.1 mL, 0.50 mmol) was added to a 3 mL toluene solution of complex 3 (22 mg, 0.028 mmol) under vigorously stirring at -78°C . After 1 h at room temperature, the resulting dark-red suspension was separated by a “trap-to-trap” technique. The solid residue was treated with an excess amount of ether solution of HCl (1.0 M, 0.3 mL). The resulting orange-red solution was evaporated to give [(C₅Me₄SiMe₃)TiCl₃] (28 mg, 0.081 mmol, 96%). The volatile part obtained in the above “trap-to-trap” separation was treated with HCl (1.0 M in ether, 0.3 mL), which led to immediate formation of NH₄Cl (2.5 mg, 0.047 mmol, 84%) as white solid.

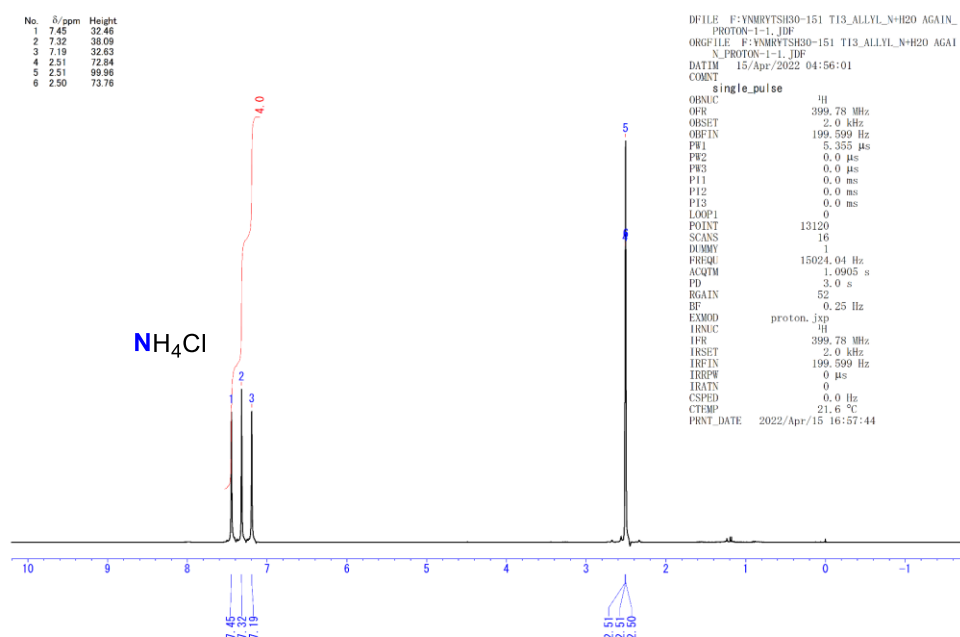


Figure S67. ¹H NMR spectrum of NH₄Cl (DMSO-*d*₆, rt).

¹H NMR monitoring of the hydrolysis of 3 with H₂O: Degassed H₂O (10 M in THF, 12 μL , 0.12 mmol) was added at room temperature to a benzene-*d*₆ solution of 3 (10.0 mg, 0.013 mmol) in the presence of 1,4-dimethoxybenzene (1.0 mg) as an internal standard. After 1 h, the formation of propane (25% NMR), and propylene (12% NMR) was confirmed by the ¹H NMR analysis. The ¹H NMR signal of NH₃ was not observed probably because it was too broad.

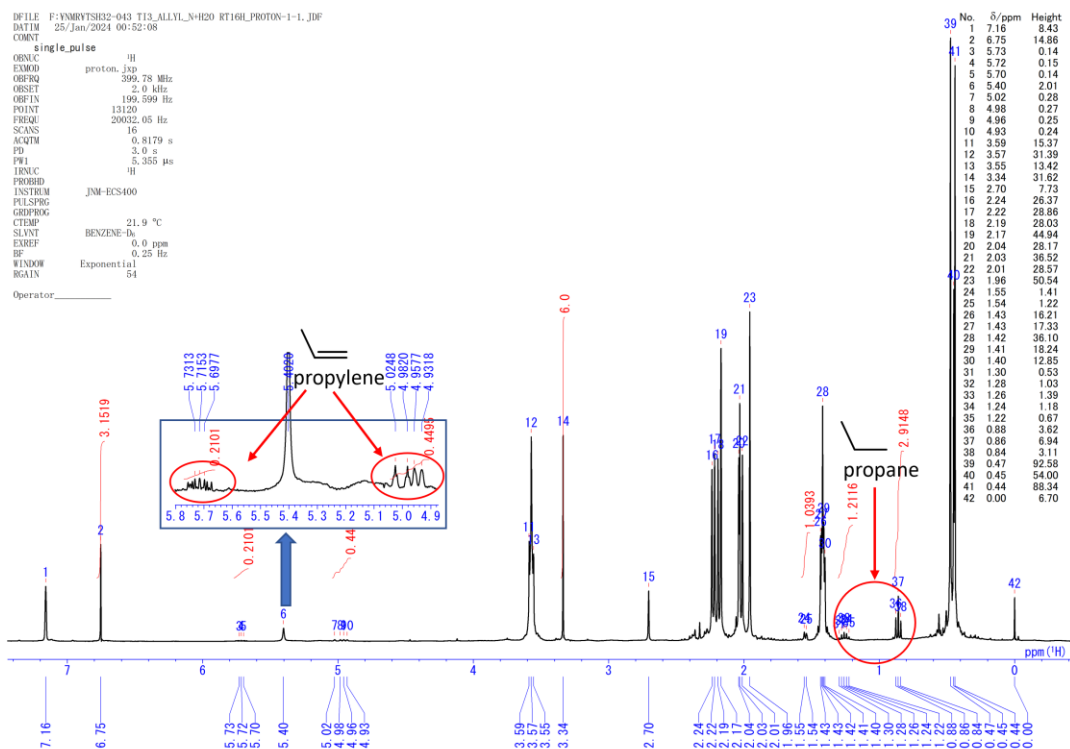


Figure S68. ^1H NMR spectrum after the hydrolysis of **3** with H_2O (C_6D_6 , rt).

Hydrolysis of **5 with H_2O :** Degassed H_2O (5.0 M in THF, 0.2 mL, 1 mmol) was added to a 5 mL toluene solution of complex **5** (41 mg, 0.052 mmol) under vigorously stirring at $-78\text{ }^\circ\text{C}$. After 1 h at room temperature, the resulting dark-red suspension was separated by a “trap-to-trap” technique. The solid residue was treated with an excess amount of ether solution of HCl (1.0 M, 0.5 mL). The resulting orange-red solution was evaporated to give $[(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{TiCl}_3]$ (46 mg, 0.13 mmol, 83%). The volatile part obtained in the above “trap-to-trap” separation was treated with HCl (1.0 M in ether, 0.5 mL), which led to immediate formation of mixture of $^i\text{PrNH}_3\text{Cl}$ (**7a**, 20% NMR) and NH_4Cl (144% NMR) as white solid (5.0 mg).

Characterization of $^i\text{PrNH}_3\text{Cl}$ (7a**):** ^1H NMR ($\text{DMSO}-d_6$, rt): δ 7.98 (brs, 3H, $(\text{CH}_3)_2\text{CHNH}_3\text{Cl}$), 3.26 (m, 1H, $(\text{CH}_3)_2\text{CHNH}_3\text{Cl}$), 1.19 (d, $J_{\text{HH}} = 6.8\text{ Hz}$, 6H, $(\text{CH}_3)_2\text{CHNH}_3\text{Cl}$). $^{13}\text{C}\{^1\text{H}\}$ NMR ($\text{DMSO}-d_6$, rt): δ 42.9 (s, $(\text{CH}_3)_2\text{CHNH}_3\text{Cl}$), 20.4 (s, $(\text{CH}_3)_2\text{CHNH}_3\text{Cl}$). EI-MS (m/z): Calculated for $\text{C}_3\text{H}_8\text{N}$ ($[\text{M}-\text{H}]^+$): 58.06567; Found. $m/z = 58.06569$ ($[\text{CH}_3\text{-CH}(\text{CH}_3)\text{-NH}]^+$), 44.04991 ($[\text{CH}_3\text{-CH-NH}_2]^+$).

Characterization of NH_4Cl : ^1H NMR ($\text{DMSO}-d_6$, rt): δ 7.39 (1:1:1 t, $J_{\text{NH}} = 51.0\text{ Hz}$, NH_4Cl).

^1H NMR monitoring of the hydrolysis of **5 with H_2O :** Degassed H_2O (10 M in THF, 10 μL , 0.10 mmol) was added at room temperature to a benzene- d_6 solution of **5** (8.0 mg, 0.010 mmol) in the presence of 1,4-dimethoxybenzene (1.0 mg) as an internal standard. After 1 h, the formation of isopropylamine (31% NMR), propane (15% NMR), and propylene (10% NMR) was confirmed by the ^1H NMR analysis.

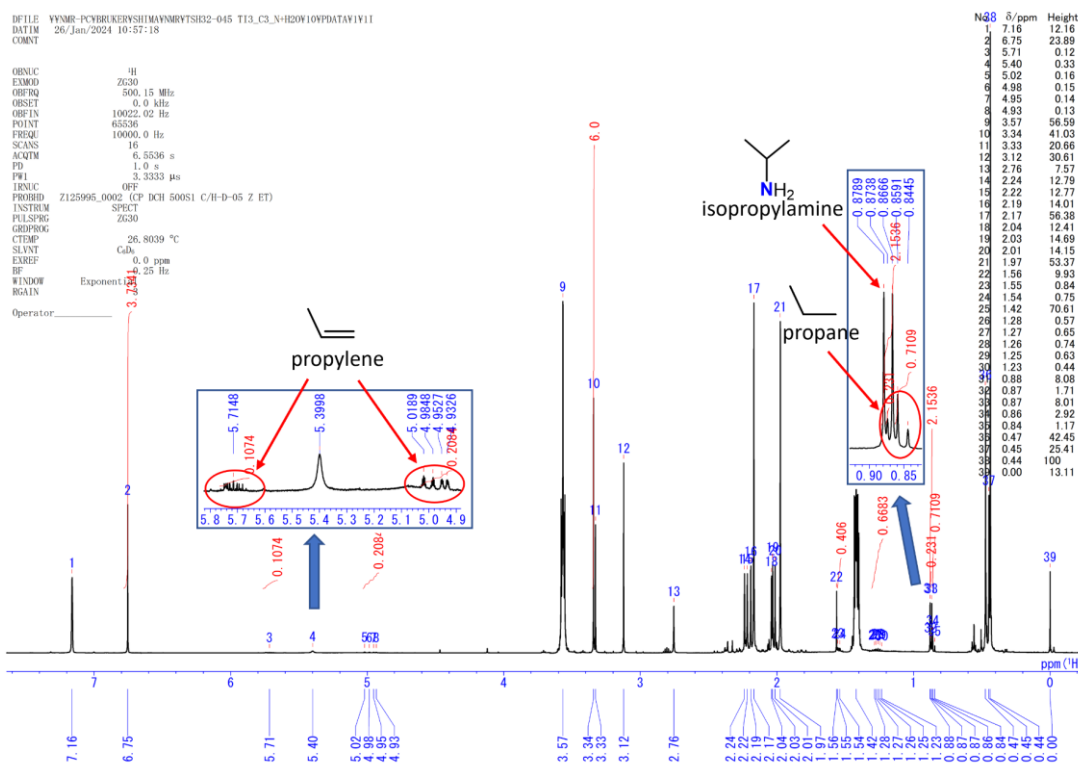


Figure S69. ^1H NMR spectrum after the hydrolysis of **5** with H_2O (C_6D_6 , rt).

Hydrolysis of ^{15}N -labelled **5- ^{15}N with H_2O :** The reaction of **5**- ^{15}N with H_2O was performed the same as that of the reaction of **5** with H_2O , leading to the formation of ^{15}N -labelled compounds $i\text{Pr}^{15}\text{NH}_3\text{Cl}$ (**7a**- ^{15}N , 31% NMR) and $^{15}\text{NH}_4\text{Cl}$ (69% NMR).

Characterization of $i\text{Pr}^{15}\text{NH}_3\text{Cl}$ (7a**- ^{15}N):** ^1H NMR ($\text{DMSO}-d_6$, rt): δ 7.98 (dd, $J_{15\text{NH}} = 72.0$ Hz, $J_{\text{HH}} = 5.6$ Hz, 3H, $(\text{CH}_3)_2\text{CH}^{15}\text{NH}_3\text{Cl}$), 3.25 (m, 1H, $(\text{CH}_3)_2\text{CH}^{15}\text{NH}_3\text{Cl}$), 1.18 (dd, $J_{\text{HH}} = 6.8$ Hz, $J_{15\text{NH}} = 2.5$ Hz, 6H, $(\text{CH}_3)_2\text{CH}^{15}\text{NH}_3\text{Cl}$). $^{13}\text{C}\{^1\text{H}\}$ NMR ($\text{DMSO}-d_6$, rt): δ 42.9 (d, $J_{15\text{NH}} = 4.5$ Hz, $(\text{CH}_3)_2\text{CH}^{15}\text{NH}_3\text{Cl}$), 20.4 (s, $(\text{CH}_3)_2\text{CH}^{15}\text{NH}_3\text{Cl}$). EI-MS: $m/z = 59.06278$ ($[\text{CH}_3\text{-CH}(\text{CH}_3)\text{-}^{15}\text{NH}]^+$), 45.04715 ($[\text{CH}_3\text{-CH-}^{15}\text{NH}_2]^+$).

Characterization of $^{15}\text{NH}_4\text{Cl}$: ^1H NMR ($\text{DMSO}-d_6$, rt): δ 7.30 (d, $J_{15\text{NH}} = 71.0$ Hz, $^{15}\text{NH}_4\text{Cl}$).

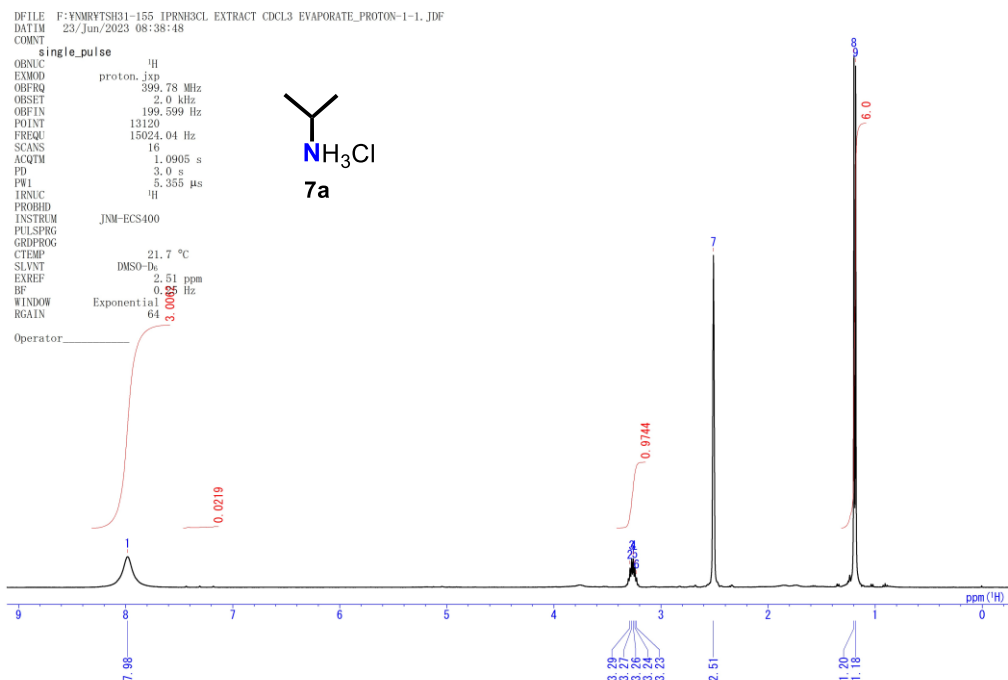


Figure S70. ¹H NMR spectrum of 7a (DMSO-d₆, rt).

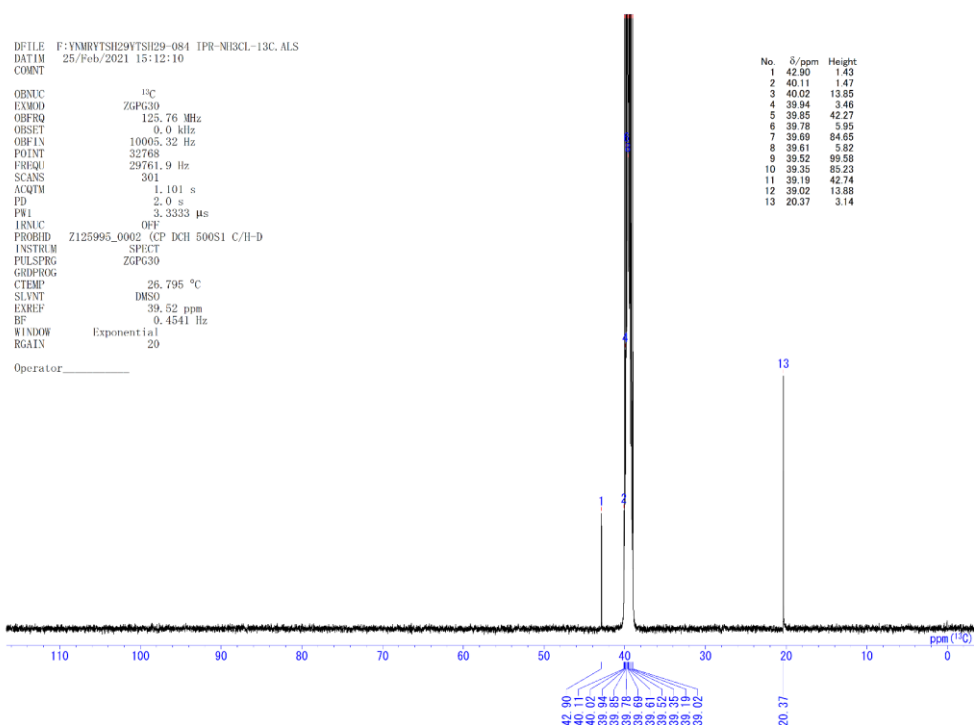


Figure S71. ¹³C{¹H} NMR spectrum of 7a (DMSO-d₆, rt).

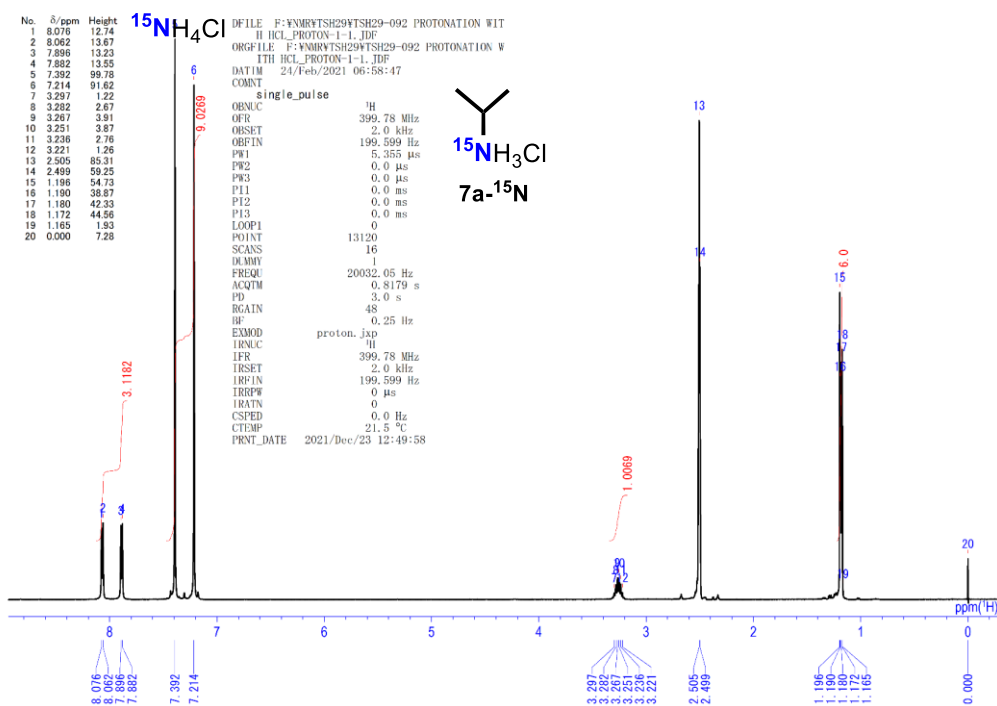


Figure S72. ^1H NMR spectrum of $7\text{a-}^{15}\text{N}$ and $^{15}\text{NH}_4\text{Cl}$ ($\text{DMSO-}d_6$, rt).

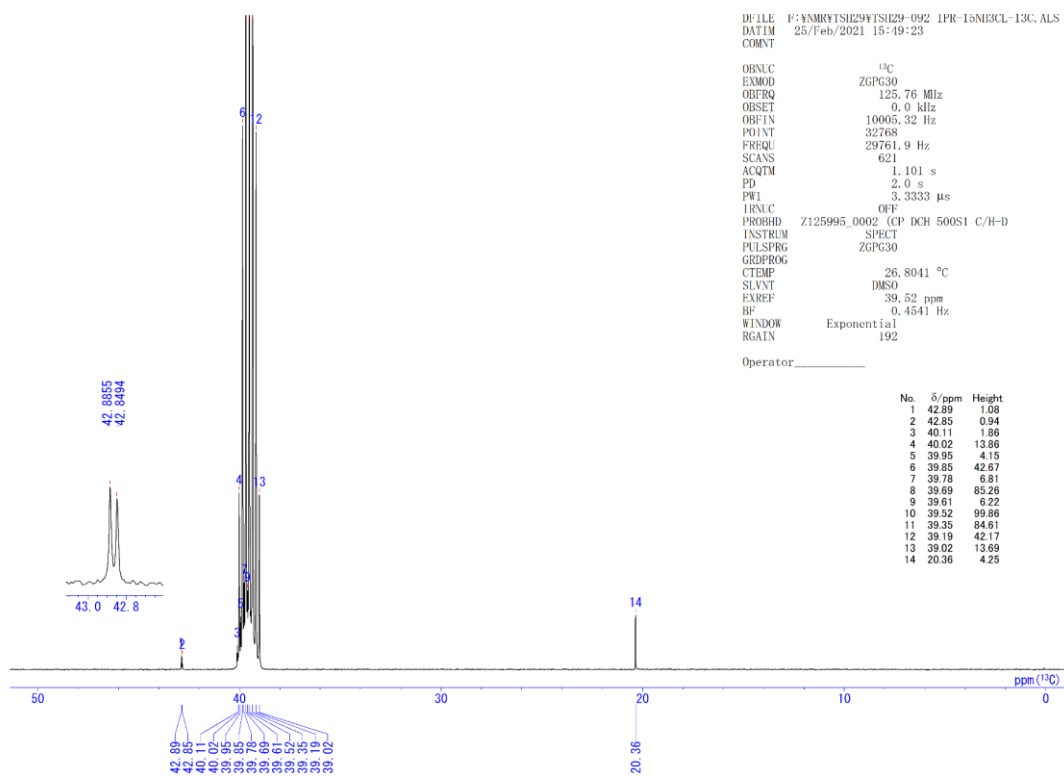


Figure S73. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of $7\text{a-}^{15}\text{N}$ ($\text{DMSO-}d_6$, rt).

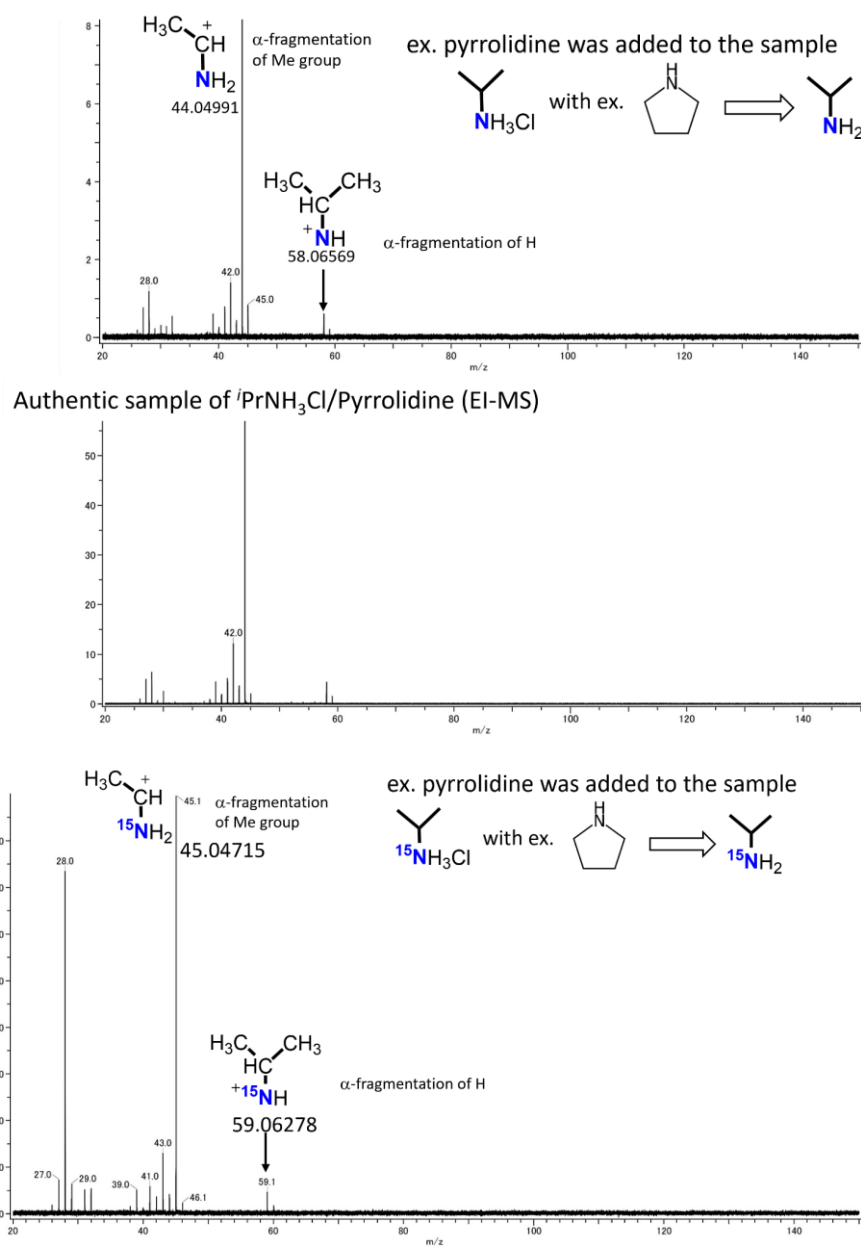
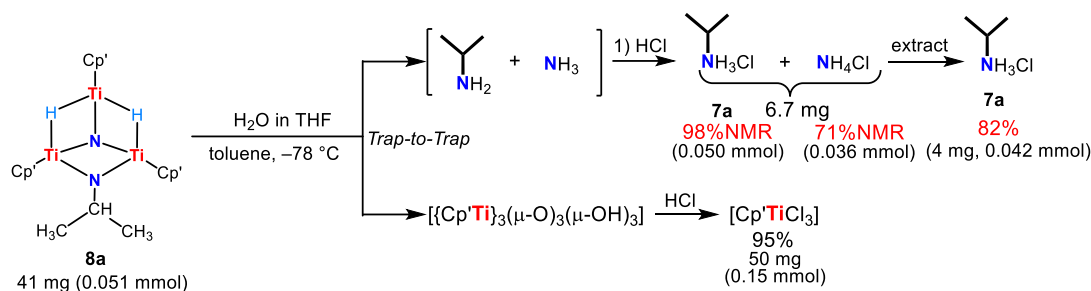


Figure S74. EI-MS spectra of **7a**, authentic sample, and **7a**- ^{15}N .

Hydrolysis of **8a** with H₂O:



Degassed H₂O (5.0 M in THF, 0.15 mL, 0.75 mmol) was added to a 5 mL toluene solution of complex **8a** (41 mg, 0.051 mmol) under vigorously stirring at -78°C . After 1 h at room temperature, the resulting dark-red suspension was separated by a “trap-to-trap” technique. The solid residue was treated with an excess amount of ether solution of HCl (1.0 M, 0.5 mL). The resulting orange-red solution was evaporated to give $[(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{TiCl}_3]$ (50 mg, 0.15 mmol, 95%). The volatile part obtained in the above “trap-to-trap” separation was treated with HCl (1.0 M in ether, 0.3 mL), which led to immediate formation of mixture of *i*PrNH₃Cl (**7a**, 98% NMR) and NH₄Cl (71% NMR) as white solid (6.7 mg). **7a** (4 mg, 0.042 mmol, 82%) was isolated by extraction with chloroform.

Calculation of NMR yields of **7a** and NH₄Cl: The total weight of a mixture of **7a** (*x* mg) and NH₄Cl (*y* mg) was 6.7 mg ($x+y=6.7$). The ¹H NMR of the mixture revealed the integration ratio of **7a** (*M_w* 95.6) and NH₄Cl (*M_w* 53.5) (**7a** ($x/95.6$) : NH₄Cl ($y/53.5$) = 1 : 0.72). From these results, *x* and *y* were calculated to be 4.8 mg (0.050 mmol, 98% NMR) and 1.9 mg (0.036 mmol, 71% NMR).

¹H NMR monitoring of the hydrolysis of **8a with H₂O:** Degassed H₂O (5.0 M in THF, 8.0 μL, 0.04 mmol) was added to a benzene-*d*₆ solution of **8a** (4.0 mg, 0.005 mmol) at room temperature. After 3 h, the formation of *i*PrNH₂ was confirmed by the ¹H NMR analysis. No free hydrocarbon units were observed in the reaction mixture.

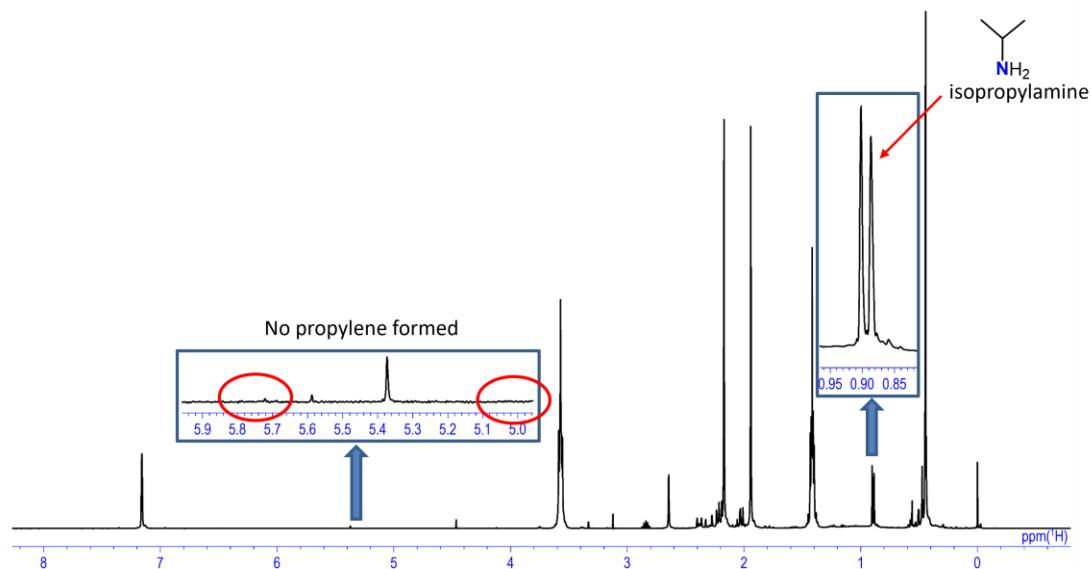
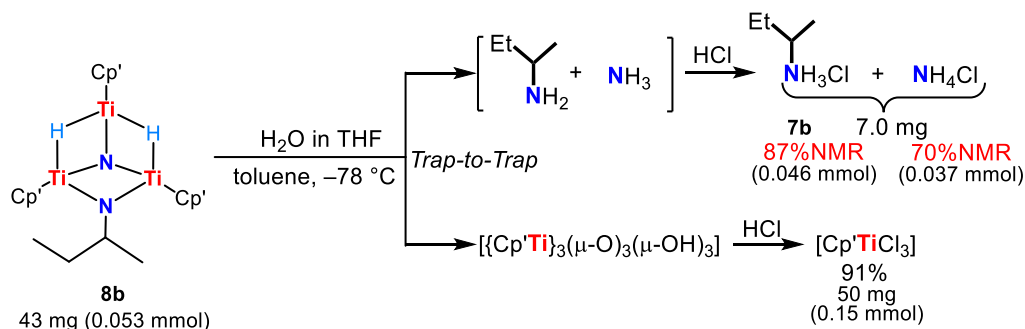


Figure S75. ^1H NMR spectrum after the hydrolysis of **8a** with H_2O (C_6D_6 , rt).

Hydrogenolysis of 8a with H_2 at high temperature: Hydrogenolysis of **8a** (10 mg, 0.015 mmol) with H_2 (4 atm) at 70°C for 1 day afforded complex **2** (80% NMR) together with free propane (83% NMR).

Protonation of 8a with HCl: HCl (1.0 M in ether, 0.1 mL) was added to a benzene- d_6 solution (0.4 mL) of **8a** (5 mg, 0.0063 mmol) at room temperature. After 1 h, the resulting orange-red solution was evaporated to give a red solid. The solid residue was dissolved in $\text{dmsO}-d_6$ and cyclohexane ($0.7\ \mu\text{L}$) was added as an internal standard. The ^1H NMR analysis revealed the formation of $i\text{PrNH}_3\text{Cl}$ (**7a**, 72% NMR) and NH_4Cl (106% NMR).

Hydrolysis of **8b** with H_2O :



Degassed H_2O (5.0 M in THF, 0.2 mL, 1 mmol) was added to a 3 mL toluene solution of complex **8b** (43 mg, 0.053 mmol) under vigorously stirring at -78°C . After 2 h at room temperature, the resulting dark-red suspension was separated by a “trap-to-trap”

technique. The solid residue was treated with an excess amount of ether solution of HCl (1.0 M in ether, 0.5 mL). The resulting orange–red solution was evaporated to give $[(C_5Me_4SiMe_3)TiCl_3]$ (50 mg, 0.15 mmol, 91%). The volatile part obtained in the above “trap-to-trap” separation was treated with HCl (1.0 M in ether, 0.3 mL), which led to immediate formation of mixture of $MeCH(CH_2CH_3)NH_3Cl$ (**7b**, 87% NMR) and NH_4Cl (70% NMR) as white solid (7 mg).

Characterization of 7b: 1H NMR (DMSO- d_6 , rt): δ 8.09 (brs, 3H, $CH_3CH(CH_2CH_3)NH_3Cl$), 3.04 (m, 1H, $CH_3CH(CH_2CH_3)NH_3Cl$), 1.64 (m, 1H, $CH_3CH(CH_2CH_3)NH_3Cl$), 1.47 (m, 1H, $CH_3CH(CH_2CH_3)NH_3Cl$), 1.17 (d, $J_{HH} = 6.4$ Hz, 3H, $CH_3CH(CH_2CH_3)NH_3Cl$), 0.89 (t, $J_{HH} = 7.5$ Hz, 3H, $CH_3CH(CH_2CH_3)NH_3Cl$). $^{13}C\{^1H\}$ NMR (DMSO- d_6 , rt): δ 48.0 (s, $CH_3CH(CH_2CH_3)NH_3Cl$), 27.1 (s, $CH_3CH(CH_2CH_3)NH_3Cl$), 17.6 (s, $CH_3CH(CH_2CH_3)NH_3Cl$), 9.7 (s, $CH_3CH(CH_2CH_3)NH_3Cl$). EI-MS (m/z): Calculated for $C_4H_{10}N$ ($[M-H]^+$): 72.0813; Found. $m/z = 72.08123$ ($[CH_3-CH_2-CH(CH_3)-NH]^+$), 58.06557 ($[CH_3-CH_2-CH-NH_2]^+$), 44.04986 ($[CH_3-CH-NH_2]^+$).

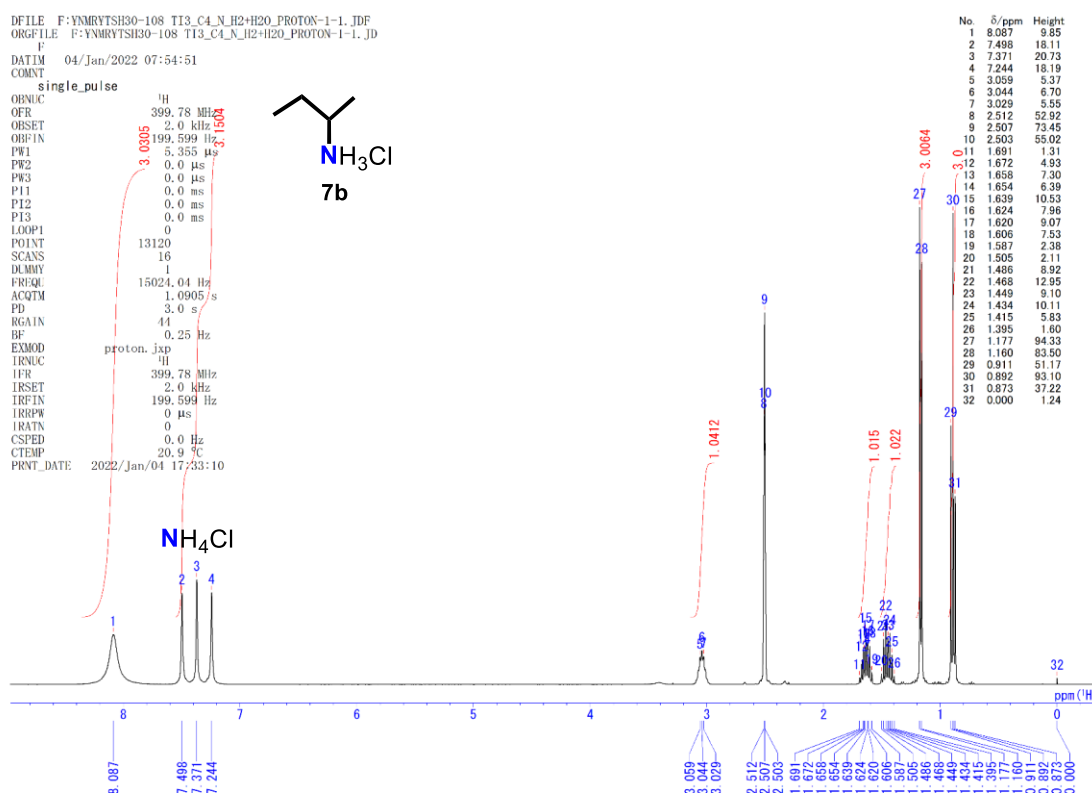


Figure S76. 1H NMR spectrum of **7b** and NH_4Cl (DMSO- d_6 , rt).

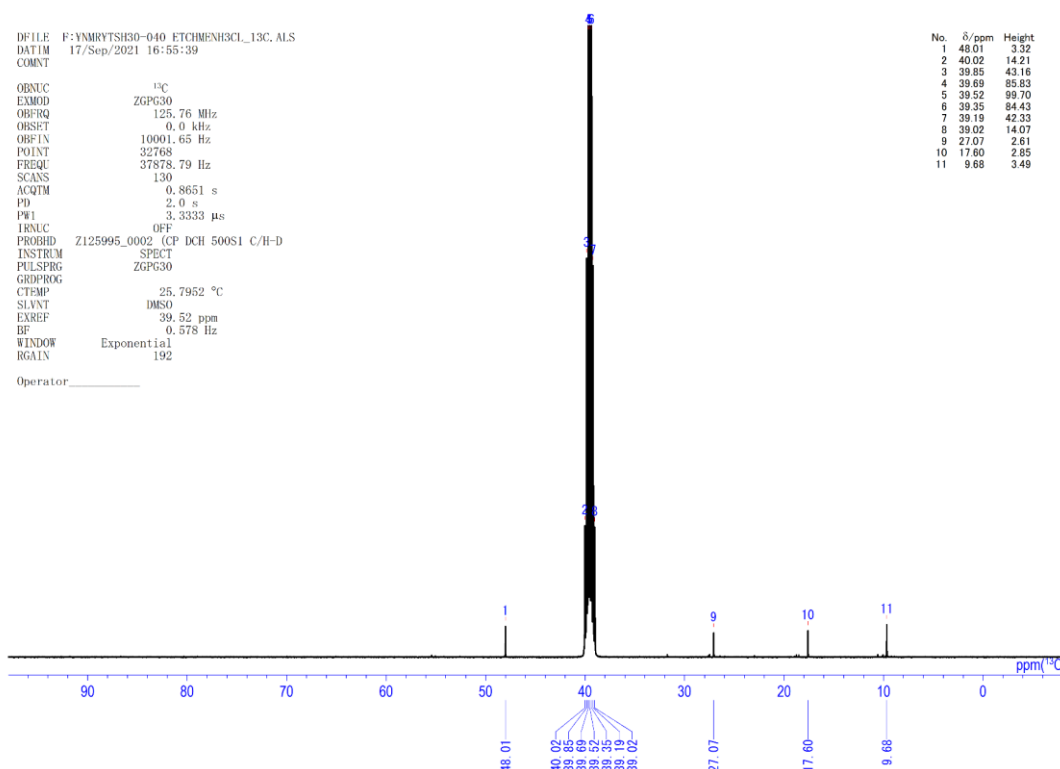
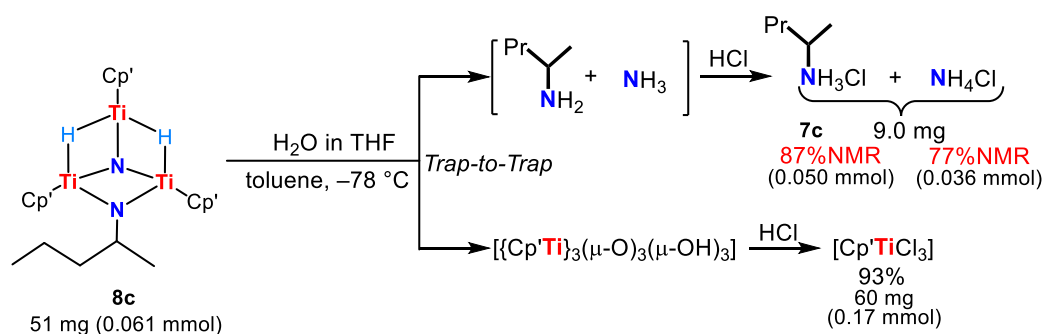


Figure S77. ¹³C NMR spectrum of **7b** (DMSO-*d*₆, rt).

Hydrolysis of **8c** with H₂O:



Degassed H₂O (5.0 M in THF, 0.2 mL, 1 mmol) was added to a 3 mL toluene solution of complex **8c** (51 mg, 0.061 mmol) under vigorously stirring at -78 °C. After 1 h at room temperature, the resulting dark-red suspension was separated by a “trap-to-trap” technique. The solid residue was treated with an excess amount of ether solution of HCl (1.0 M in ether, 0.5 mL). The resulting orange-red solution was evaporated to give [(C₅Me₄SiMe₃)TiCl₃] (60 mg, 0.17 mmol, 93%). The volatile part obtained in the above “trap-to-trap” separation was treated with HCl (1.0 M in ether, 0.3 mL), which led to immediate formation of mixture of MeCH(CH₂CH₂CH₃)NH₃Cl (**7c**, 87% NMR) and NH₄Cl (77% NMR) as white solid (9 mg).

Characterization of 7c: ¹H NMR (DMSO-*d*₆, rt): δ 8.13 (brs, 3H, CH₃CH(CH₂CH₂CH₃)NH₃Cl), 3.11 (m, 1H, CH₃CH(CH₂CH₂CH₃)NH₃Cl), 1.58 (m, 1H, CH₃CH(CH₂CH₂CH₃)NH₃Cl), 1.33 (m, 3H, CH₃CH(CH₂CH₂CH₃)NH₃Cl), 1.18 (d, *J*_{HH} = 6.5 Hz, 3H, CH₃CH(CH₂CH₂CH₃)NH₃Cl), 0.88 (t, *J*_{HH} = 7.1 Hz, 3H,

CH₃CH(CH₂CH₂CH₃)NH₃Cl). ¹³C{¹H} NMR (DMSO-*d*₆, rt): δ 46.5 (s, CH₃CH(CH₂CH₂CH₃)NH₃Cl), 36.2 (s, CH₃CH(CH₂CH₂CH₃)NH₃Cl), 18.1₂ (s, CH₃CH(CH₂CH₂CH₃)NH₃Cl), 18.0₇ (s, CH₃CH(CH₂CH₂CH₃)NH₃Cl), 13.7 (s, CH₃CH(CH₂CH₂CH₃)NH₃Cl). EI-MS (*m/z*): Calculated for C₅H₁₂N ([M-H]⁺): 86.09697; Found. *m/z* = 86.09692 ([CH₃-(CH₂)₂-CH(CH₃)-NH]⁺), 72.08113 ([CH₃-(CH₂)₂-CH-NH₂]⁺), 44.04980 ([CH₃-CH-NH₂]⁺).

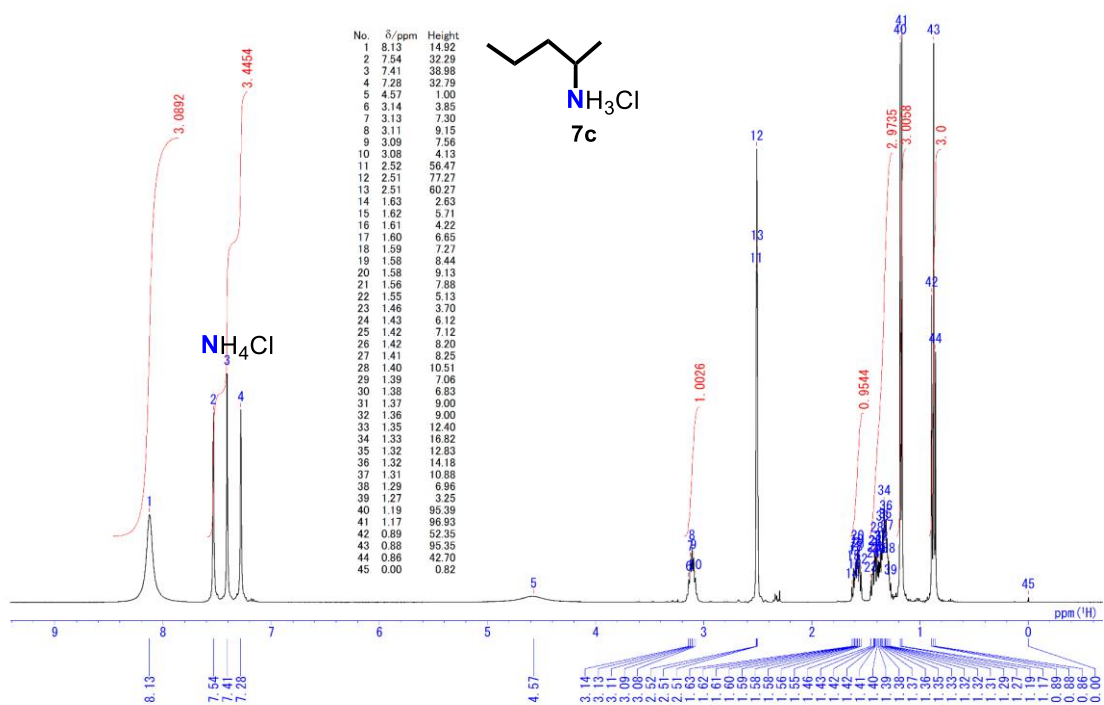


Figure S78. ¹H NMR spectrum of 7c and NH₄Cl (DMSO-*d*₆, rt).

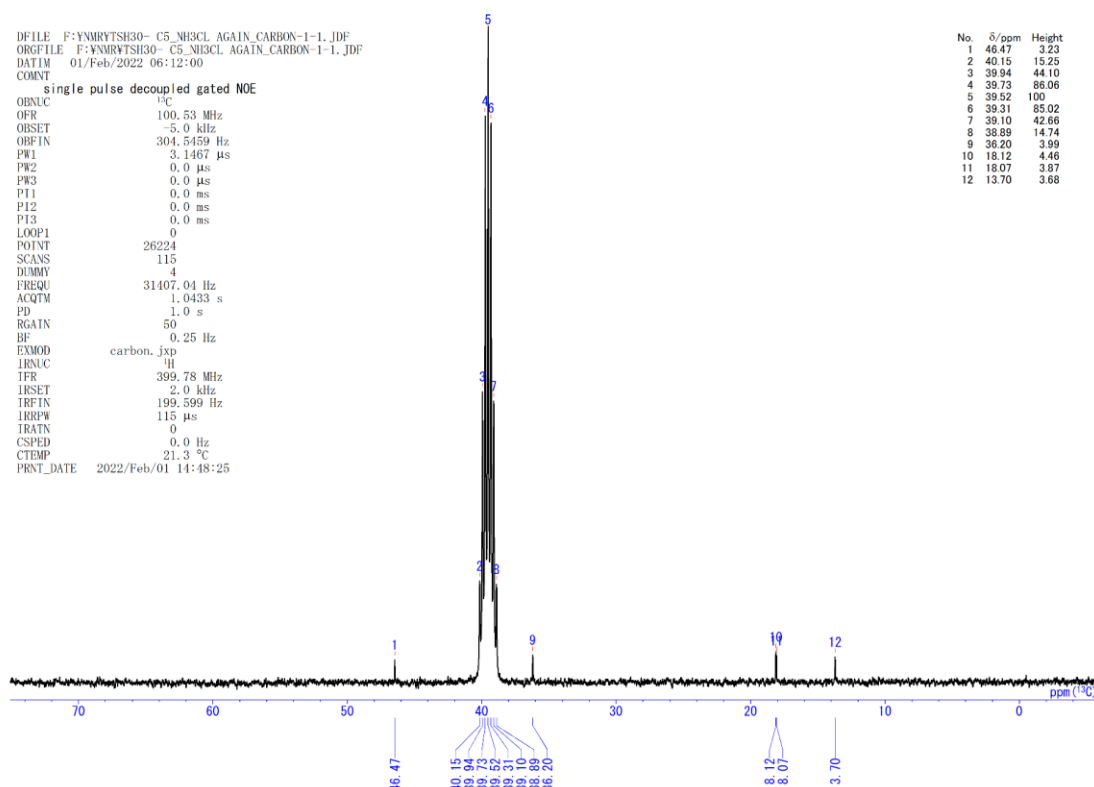
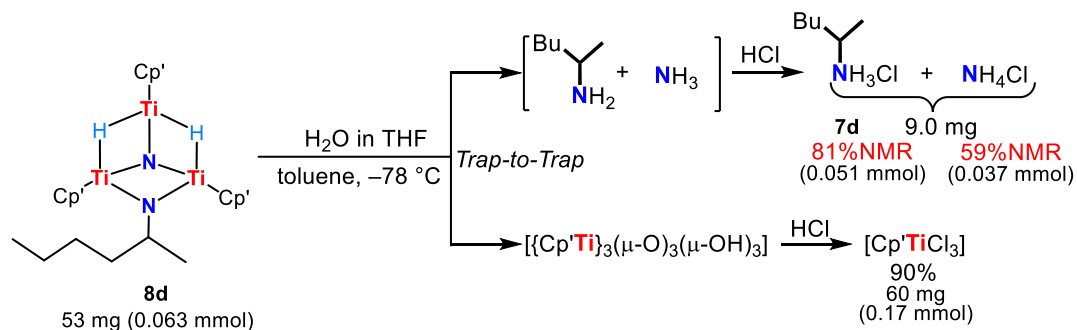


Figure S79. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **7c** ($\text{DMSO}-d_6$, rt).

Hydrolysis of **8d** with H_2O :



Degassed H_2O (5.0 M in THF, 0.2 mL, 1 mmol) was added to a 3 mL toluene solution of complex **8d** (53 mg, 0.063 mmol) under vigorously stirring at -78°C . After 2 h at room temperature, the resulting dark-red suspension was separated by a “trap-to-trap” technique. The solid residue was treated with an excess amount of ether solution of HCl (1.0 M in ether, 0.6 mL). The resulting orange-red solution was evaporated to give $[(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{TiCl}_3]$ (60 mg, 0.17 mmol, 90%). The volatile part obtained in the above “trap-to-trap” separation was treated with HCl (1.0 M in ether, 0.3 mL), which led to immediate formation of mixture of $\text{MeCH}(\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3)\text{NH}_3\text{Cl}$ (**7d**, 81% NMR) and NH_4Cl (59% NMR) as white solid (9.0 mg).

Characterization of 7d: ^1H NMR ($\text{DMSO}-d_6$, rt): δ 8.13 (brs, 3H, $\text{CH}_3\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3)\text{NH}_3\text{Cl}$), 3.09 (m, 1H, $\text{CH}_3\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3)\text{NH}_3\text{Cl}$), 1.61 (m, 1H, $\text{CH}_3\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3)\text{NH}_3\text{Cl}$), 1.43 (m, 1H,

CH₃CH(CH₂CH₂CH₂CH₃)NH₃Cl), 1.28 (m, 4H, CH₃CH(CH₂CH₂CH₂CH₃)NH₃Cl), 1.18 (d, $J_{\text{HH}} = 6.4$ Hz, 3H, CH₃CH(CH₂CH₂CH₂CH₃)NH₃Cl), 0.88 (t, $J_{\text{HH}} = 7.2$ Hz, 3H, CH₃CH(CH₂CH₂CH₂CH₃)NH₃Cl). ¹³C{¹H} NMR (DMSO-*d*₆, rt): δ 46.7 (s, CH₃CH(CH₂CH₂CH₂CH₃)NH₃Cl), 33.8 (s, CH₃CH(CH₂CH₂CH₂CH₃)NH₃Cl), 26.9 (s, CH₃CH(CH₂CH₂CH₂CH₃)NH₃Cl), 21.9 (s, CH₃CH(CH₂CH₂CH₂CH₃)NH₃Cl), 18.1 (s, CH₃CH(CH₂CH₂CH₂CH₃)NH₃Cl), 13.8 (s, CH₃CH(CH₂CH₂CH₂CH₃)NH₃Cl). EI-MS (*m/z*): Calculated for C₆H₁₄N ([M-H]⁺): 100.1126; Found. *m/z* = 100.1125 ([CH₃-(CH₂)₃-CH(CH₃)-NH]⁺), 86.09685 ([CH₃-(CH₂)₃-CH-NH₂]⁺), 44.04979 ([CH₃-CH-NH₂]⁺).

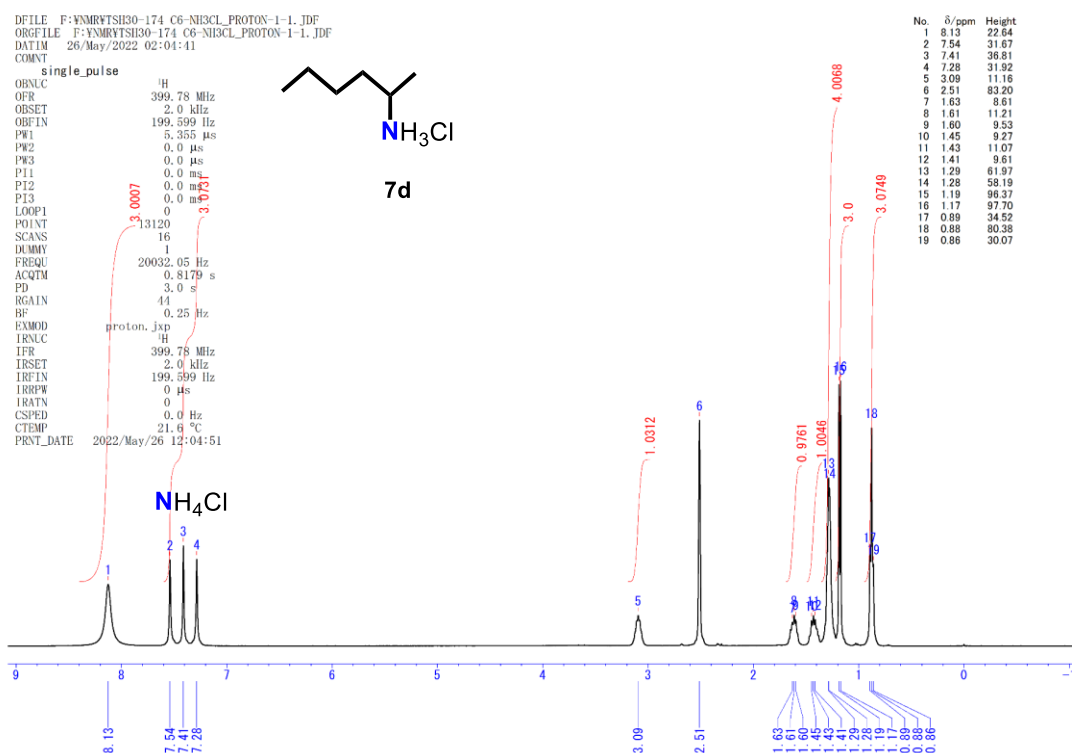


Figure S80. ¹H NMR spectrum of 7d and NH₄Cl (DMSO-*d*₆, rt).

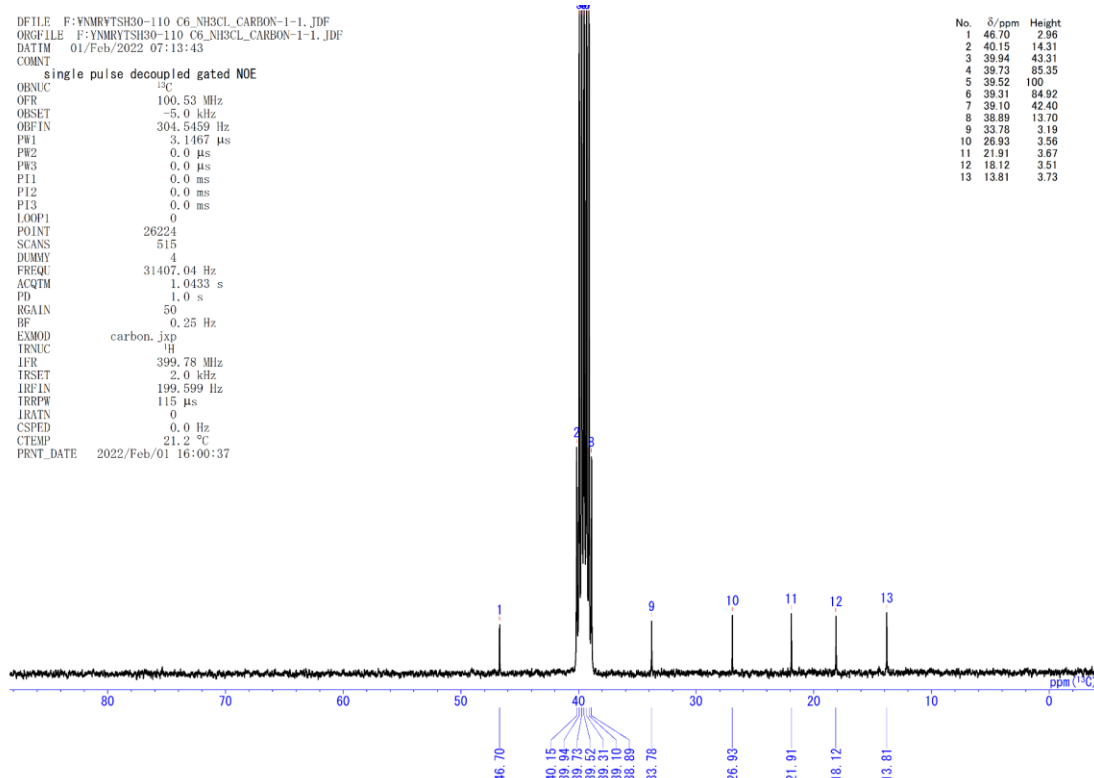
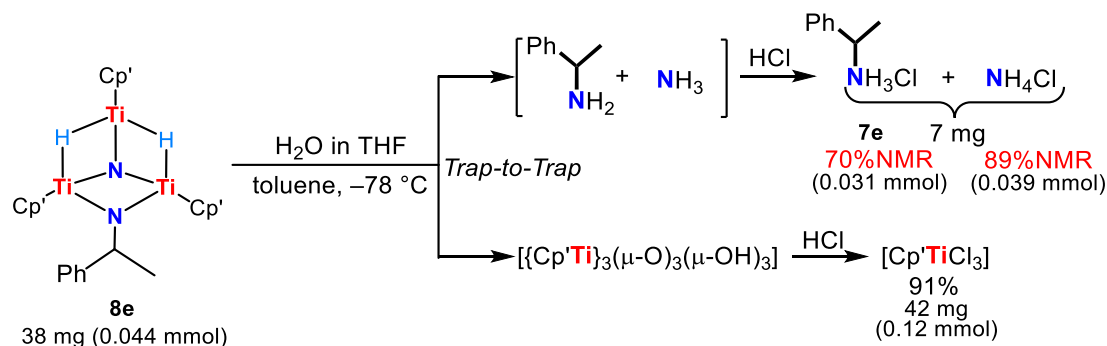


Figure S81. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **7d** (DMSO- d_6 , rt).

Hydrolysis of **8e** with H_2O :



Degassed H_2O (5.0 M in THF, 0.2 mL, 1.0 mmol) was added to a 3 mL toluene solution of complex **8e** (38 mg, 0.044 mmol) under vigorously stirring at -78°C . After 2 h at room temperature, the resulting dark-red suspension was separated by a “trap-to-trap” technique. The solid residue was treated with an excess amount of ether solution of HCl (1.0 M in ether, 0.6 mL). The resulting orange-red solution was evaporated to give $[(\text{C}_5\text{Me}_4\text{SiMe}_3)\text{TiCl}_3]$ (42 mg, 0.12 mmol, 91%). The volatile part obtained in the above “trap-to-trap” separation was treated with HCl (1.0 M in ether, 0.3 mL), which led to immediate formation of mixture of $\text{MeCHPhNH}_3\text{Cl}$ (**7e**, 70% NMR) and NH_4Cl (89% NMR) as white solid (7 mg).

Characterization of 7e: ^1H NMR (DMSO- d_6 , rt): δ 8.60 (brs, 3H, $\text{CH}_3\text{CHPhNH}_3\text{Cl}$), 7.54-7.36 (5H, Ph overlap with NH_4Cl), 4.37 (m, 1H, $\text{CH}_3\text{CHPhNH}_3\text{Cl}$), 1.52 (d, $J_{\text{HH}} =$

6.7 Hz, 3H, CH₃CHPhNH₃Cl). ¹³C{¹H} NMR (DMSO-*d*₆, rt): δ 139.5 (s, Ph), 128.6 (s, Ph), 128.3 (s, Ph), 126.9 (s, Ph), 50.0 (s, CH₃CHPhNH₃Cl), 20.8 (s, CH₃CHPhNH₃Cl). EI-MS (*m/z*): Calculated for C₈H₁₀N ([M-H]⁺): 120.0813; Found. *m/z* = 120.0811 ([C₆H₅-CH(CH₃)-NH]⁺), 106.0655 ([C₆H₅-CH-NH₂]⁺).

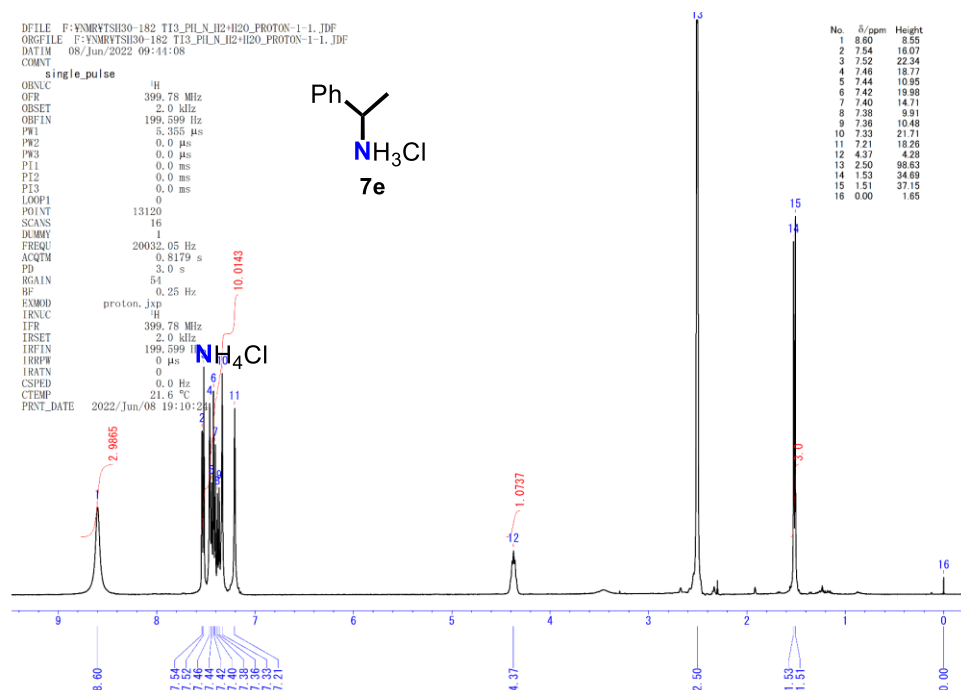


Figure S82. ¹H NMR spectrum of 7e and NH₄Cl (DMSO-*d*₆, rt).

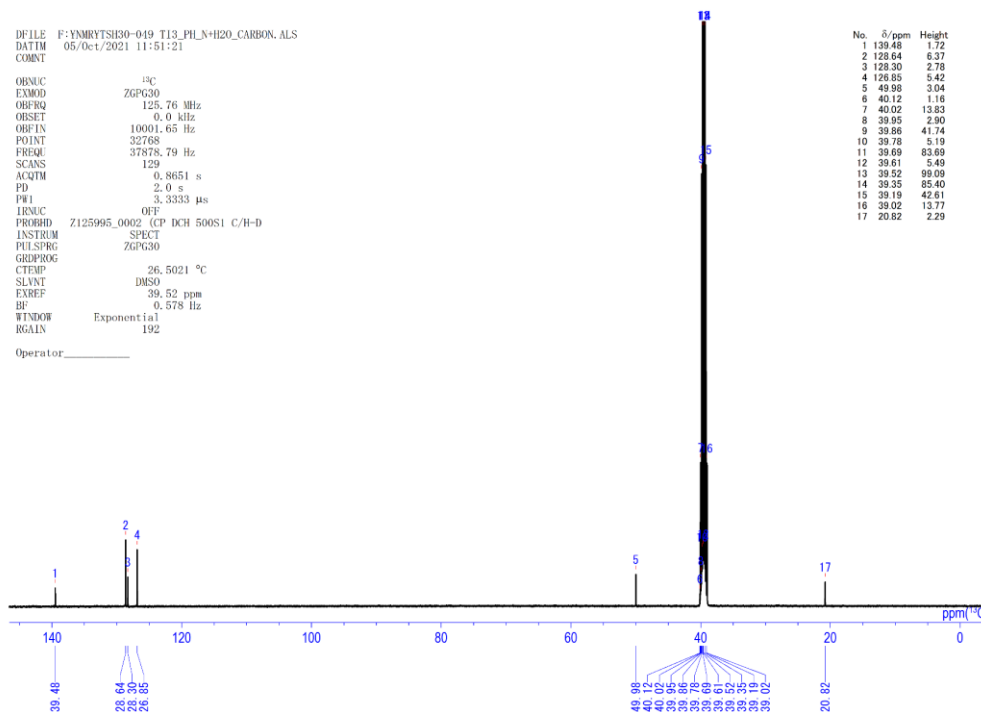
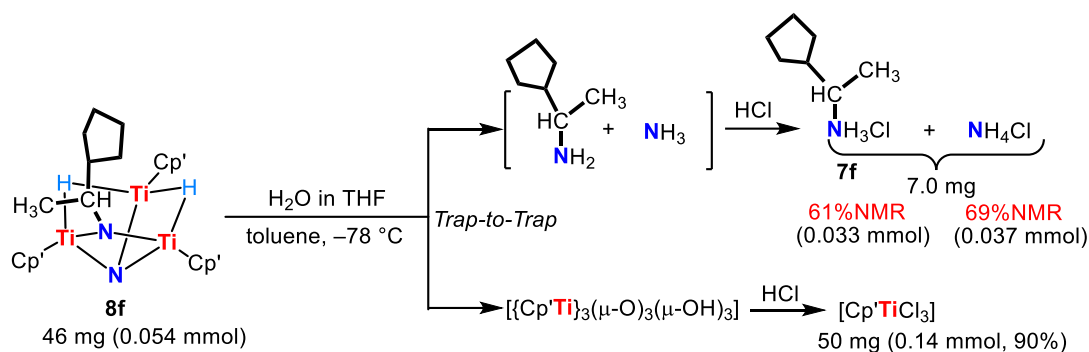


Figure S83. ¹³C{¹H} NMR spectrum of 7e (DMSO-*d*₆, rt).

Hydrolysis of **8f** with H₂O:



Degassed H₂O (5.0 M in THF, 0.3 mL, 1.5 mmol) was added to a 3 mL toluene solution of complex **8f** (46 mg, 0.054 mmol) under vigorously stirring at -78 °C. After 2 h at room temperature, the resulting dark-red suspension was separated by a "trap-to-trap" technique. The solid residue was treated with an excess amount of ether solution of HCl (1.0 M in ether, 0.6 mL). The resulting orange-red solution was evaporated to give [(C₅Me₄SiMe₃)TiCl₃] (50 mg, 0.14 mmol, 90%). The volatile part obtained in the above "trap-to-trap" separation was treated with HCl (1.0 M in ether, 0.5 mL), which led to immediate formation of mixture of C₅H₉CH(CH₃)NH₃Cl (**7f**, 61% NMR) and NH₄Cl (69% NMR) as white solid (7.0 mg).

Characterization of 7f: ¹H NMR (DMSO-*d*₆, rt): δ 8.06 (brs, 3H, C₅H₉CH(CH₃)NH₃Cl), 2.95 (m, 1H, C₅H₉CH(CH₃)NH₃Cl), 1.91 (m, 1H, C₅H₉CH(CH₃)NH₃Cl), 1.71 (m, 2H, C₅H₉CH(CH₃)NH₃Cl), 1.54 (m, 2H, C₅H₉CH(CH₃)NH₃Cl), 1.48 (m, 2H, C₅H₉CH(CH₃)NH₃Cl), 1.24 (m, 2H, C₅H₉CH(CH₃)NH₃Cl), 1.17 (d, *J*_{HH} = 6.1 Hz, 3H, C₅H₉CH(CH₃)NH₃Cl). ¹³C{¹H} NMR (DMSO-*d*₆, rt): δ 51.1 (s, C₅H₉CH(CH₃)NH₃Cl), 43.9 (s, C₅H₉CH(CH₃)NH₃Cl), 29.2 (s, C₅H₉CH(CH₃)NH₃Cl), 28.6 (s, C₅H₉CH(CH₃)NH₃Cl), 24.9 (s, C₅H₉CH(CH₃)NH₃Cl), 24.8 (s, C₅H₉CH(CH₃)NH₃Cl), 17.4 (s, C₅H₉CH(CH₃)NH₃Cl). EI-MS (*m/z*): Calculated for C₇H₁₄N ([M-H]⁺): 112.1126; Found. *m/z* = 112.1128 ([C₅H₉-CH(CH₃)-NH]⁺), 98.0968 ([C₅H₉-CH-NH₂]⁺), 44.04981 ([CH₃-CH-NH₂]⁺).

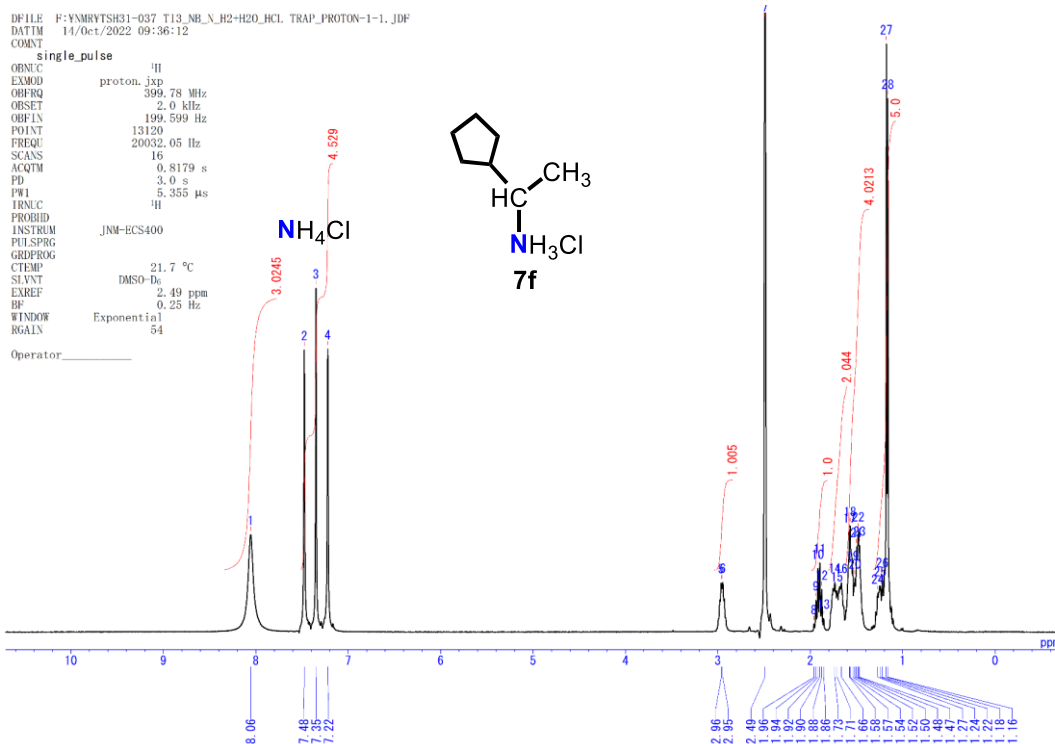


Figure S84. ¹H NMR spectrum of 7f and NH₄Cl (DMSO-*d*₆, rt).

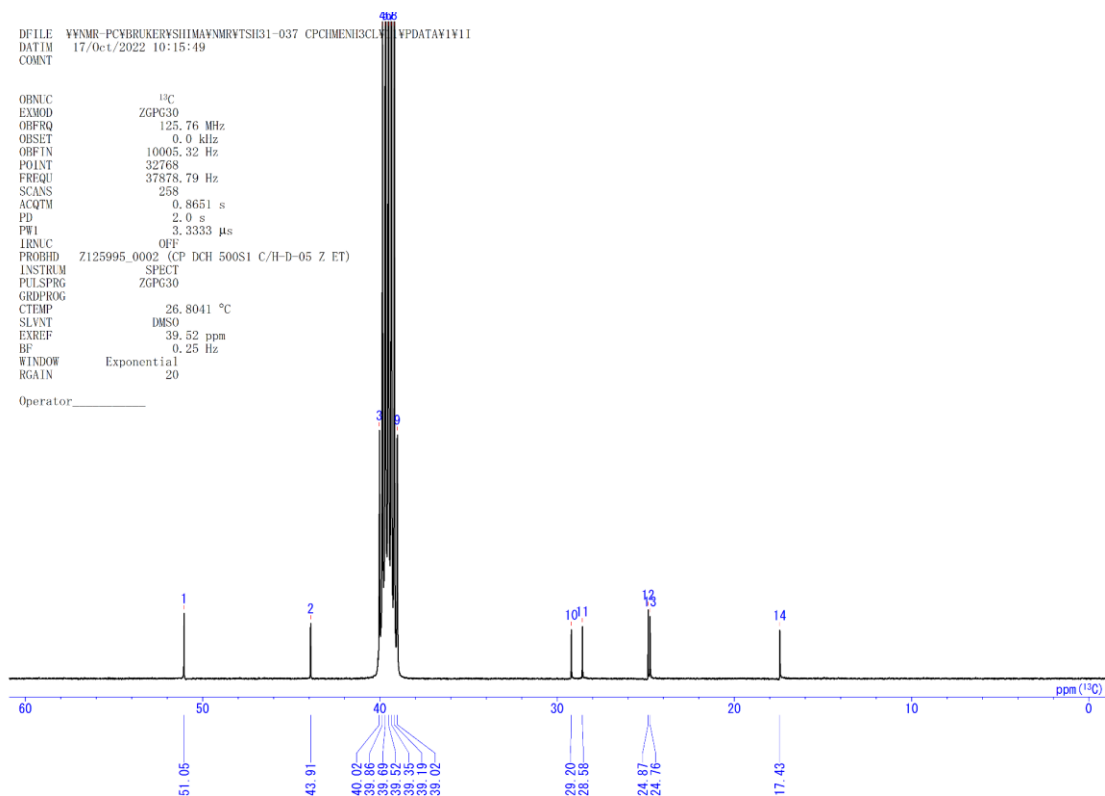
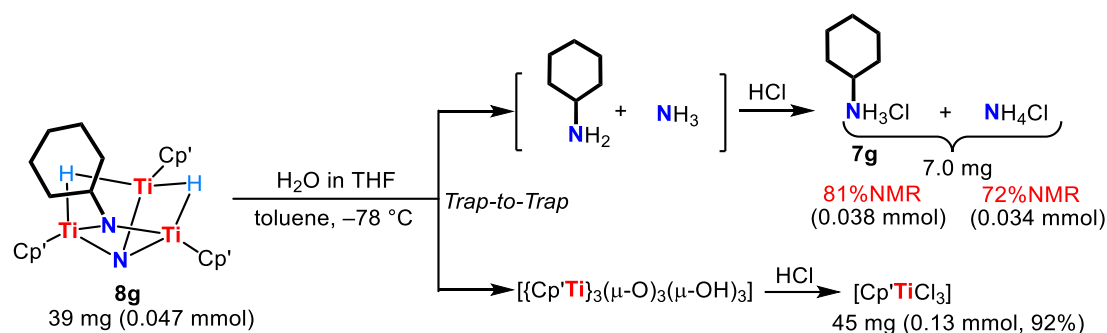


Figure S85. ¹³C{¹H} NMR spectrum of 7f (DMSO-*d*₆, rt).

Hydrolysis of **8g** with H₂O:



Degassed H₂O (5.0 M in THF, 0.3 mL, 1.5 mmol) was added to a 3 mL toluene solution of complex **8g** (39 mg, 0.047 mmol) under vigorously stirring at -78 °C. After 2 h at room temperature, the resulting dark-red suspension was separated by a "trap-to-trap" technique. The solid residue was treated with an excess amount of ether solution of HCl (1.0 M in ether, 0.6 mL). The resulting orange-red solution was evaporated to give [(C₅Me₄SiMe₃)TiCl₃] (45 mg, 0.13 mmol, 92%). The volatile part obtained in the above "trap-to-trap" separation was treated with HCl (1.0 M in ether, 0.5 mL), which led to immediate formation of mixture of C₆H₁₁NH₃Cl (**7g**, 81% NMR) and NH₄Cl (72% NMR) as white solid (7.0 mg).

Characterization of **7g:** ¹H NMR (DMSO-*d*₆, rt): δ 8.09 (brs, 3H, C₆H₁₁NH₃Cl), 2.91 (m, 1H, C₆H₁₁NH₃Cl), 1.90 (m, 2H, C₆H₁₁NH₃Cl), 1.71 (m, 2H, C₆H₁₁NH₃Cl), 1.56 (m, 1H, C₆H₁₁NH₃Cl), 1.25 (m, 4H, C₆H₁₁NH₃Cl), 1.09 (m, 1H, C₆H₁₁NH₃Cl). ¹³C{¹H} NMR (DMSO-*d*₆, rt): δ 49.2 (s, C₅H₁₁NH₃Cl), 30.3 (s, C₅H₁₁NH₃Cl), 24.6 (s, C₅H₁₁NH₃Cl), 23.7 (s, C₅H₁₁NH₃Cl). EI-MS (*m/z*): Calculated for C₆H₁₃N ([M]⁺): 99.1048; Found. 99.1047.

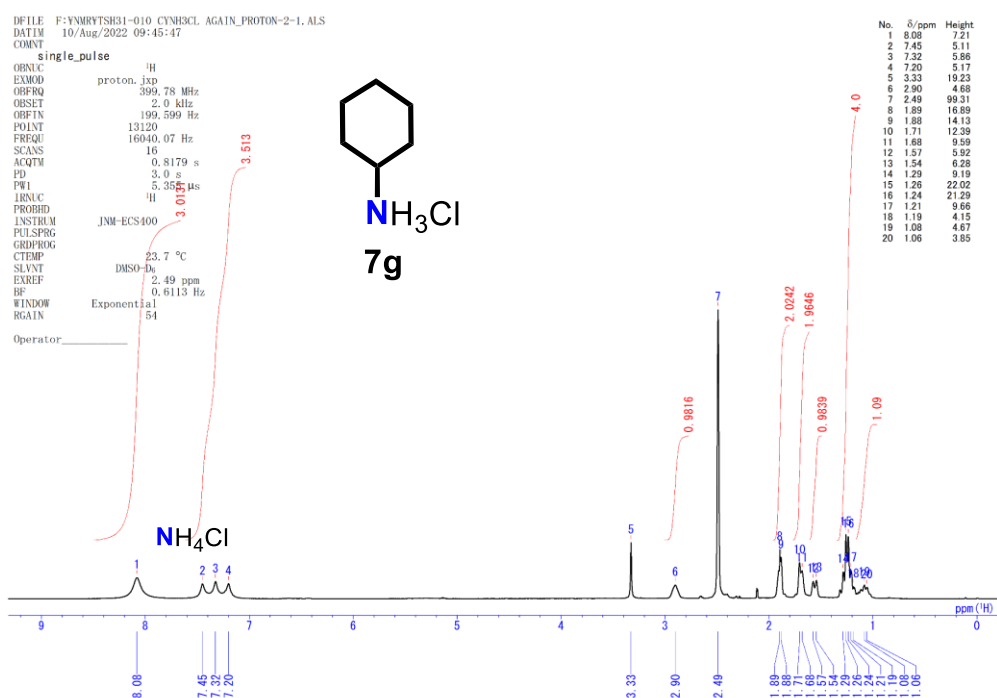


Figure S86. ¹H NMR spectrum of **7g** and NH₄Cl (DMSO-*d*₆, rt).

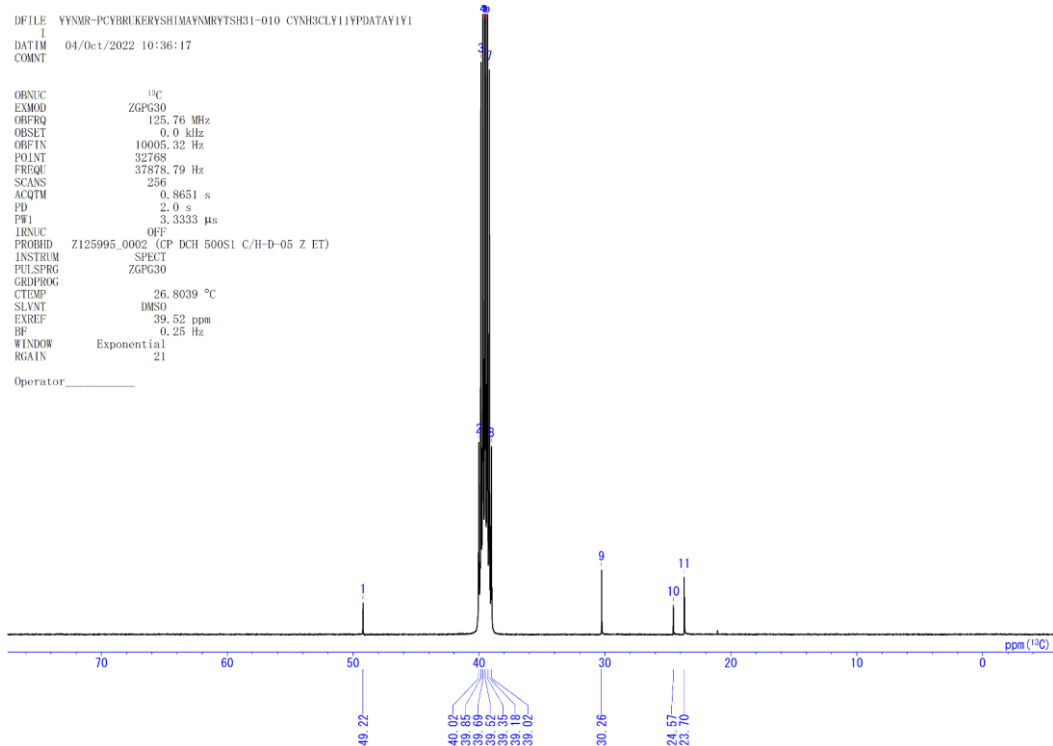


Figure S87. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **7g** (DMSO- d_6 , rt).

3. Kinetic studies

General procedure for kinetic studies of the reaction of 4a with N₂: In a typical experiment, a 5-mm pressure NMR tube (Wilmad Lab Glass) was charged with **4a** (5 mg, 0.0065 mmol) and C₆D₆ (0.40 mL, 16 mM) in a glovebox. The solution was degassed under vacuum. High pressure N₂ gas (5 atm) was then introduced to the NMR tube. After vigorously shaking at room temperature, **4a** was quantitatively converted to **6**. The sample was heated at various temperatures and analyzed by using an NMR spectrometer. The relative concentration was calculated based on the integration of the resonances of the C₅Me₄SiMe₃ groups in the C₅Me₄SiMe₃ ligands.

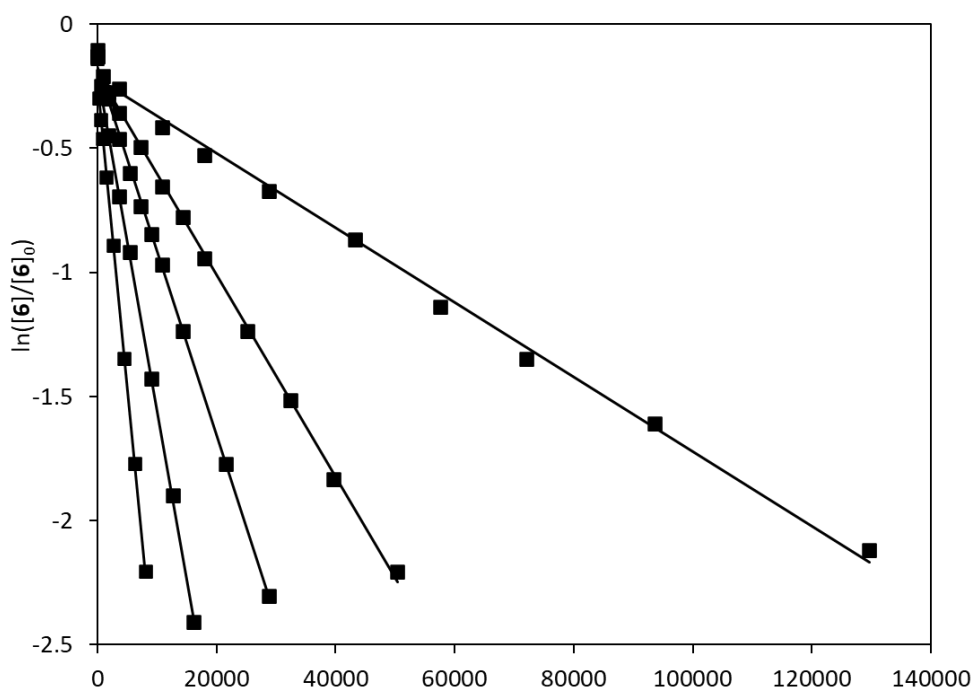


Figure S88. First-order plots of the disappearance of **6** as a function of time (s) at different temperature.

Table S1. Observed rate constants (k_{obs}) for the conversion of **6** to **5**.

Temperature °C (K)	k_{obs} (s ⁻¹)
22 °C (295 K)	1.50448×10^{-5}
30 °C (303 K)	4.07468×10^{-5}
35 °C (308 K)	7.44581×10^{-5}
40 °C (313 K)	1.36892×10^{-4}
45 °C (318 K)	2.47584×10^{-4}

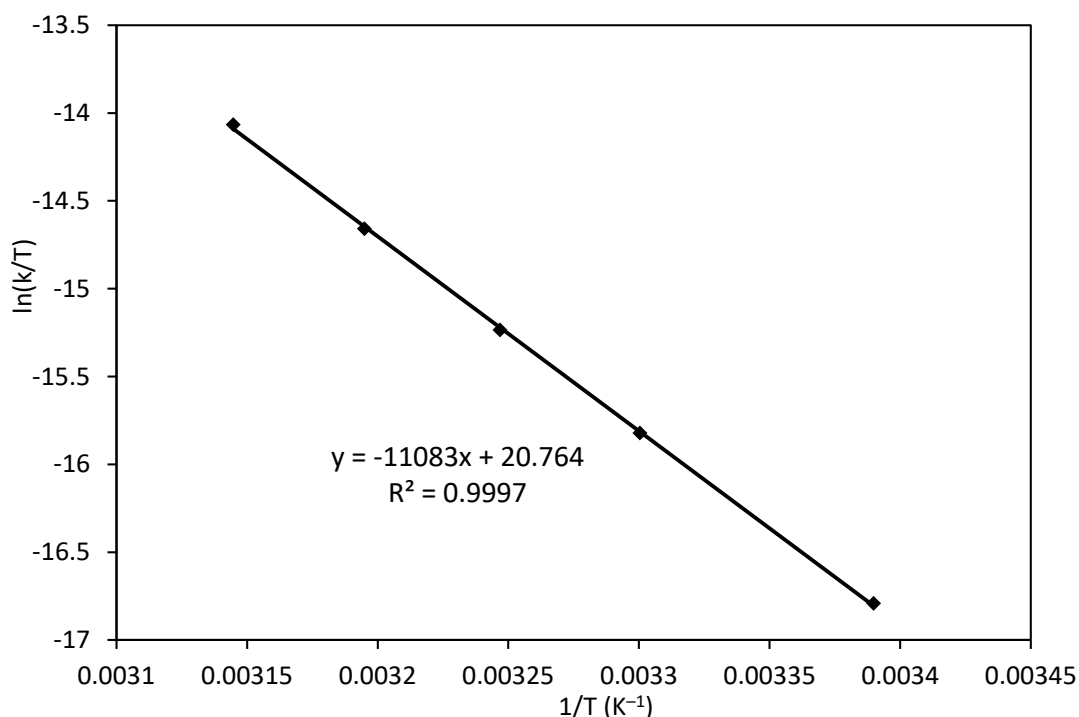


Figure S89. Eyring plot of the conversion of **6**.

The activation parameters for the reaction of **4a** with N₂ (5 atm) were determined by measuring rate constants at various temperatures (Fig. S88). An Eyring plot (Fig. S89) was constructed from these data (Table S1), and the activation enthalpy and entropy were extracted as follows: $\Delta H^\ddagger = 22.0(2)$ kcal/mol, $\Delta S^\ddagger = -5.9(7)$ eu, $\Delta G^\ddagger(298\text{K}) = 23.7$ kcal/mol.

General procedure for kinetic studies of the conversion of 5 to 3: 5-mm J. Young NMR tube was charged with **5** (3.0 mg $\times$ 5, 0.0038 $\times$ 5 mmol) and C₆D₆ (0.40 mL $\times$ 5, 0.01 M) in a glovebox. The solution of **5** was heated at various temperatures, and analyzed by using an NMR spectrometer. The relative concentration was calculated based on the integration of the resonances of the C₅Me₄SiMe₃ groups in the C₅Me₄SiMe₃ ligands.

Table S2. Observed rate constants (k_{obs}) for the conversion of **5** to **3**.

Temperature °C (K)	k_{obs} (s ⁻¹)
60 °C (333 K)	2.67266×10^{-5}
65 °C (338 K)	4.57702×10^{-5}
70 °C (343 K)	7.83415×10^{-5}
75 °C (348 K)	1.29236×10^{-4}
80 °C (353 K)	2.11049×10^{-4}
65 °C (338 K)	* 3.40168×10^{-5}

* conversion of **5-d** to **3-d**.

Kinetic isotope effect (KIE) = $k_{\text{H}}/k_{\text{D}} = 4.57702 \times 10^{-5} / 3.40168 \times 10^{-5} = 1.35$

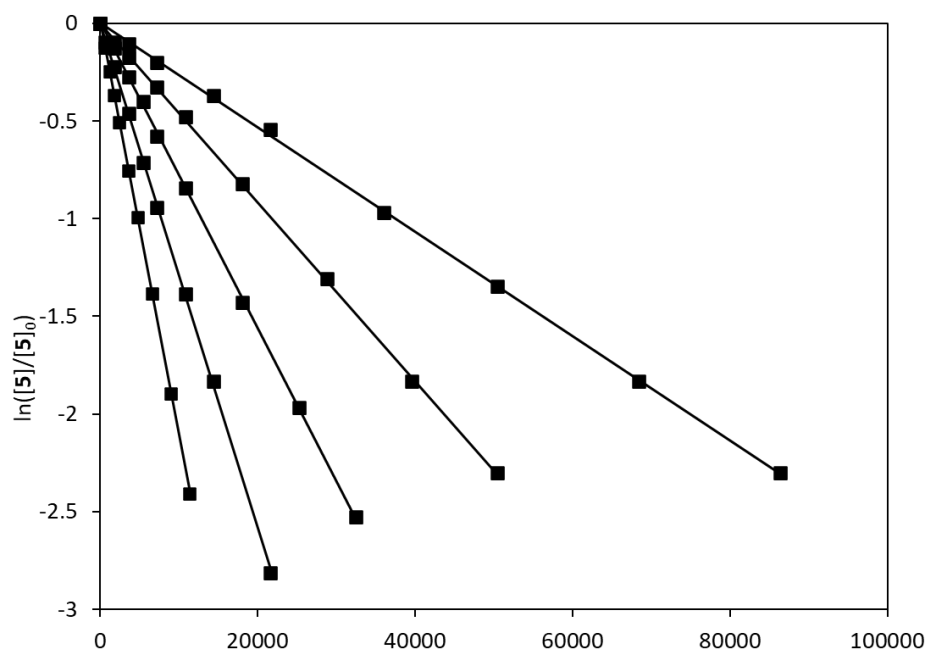


Figure S90. First-order plots of the disappearance of **5** as a function of time (s) at different temperature.

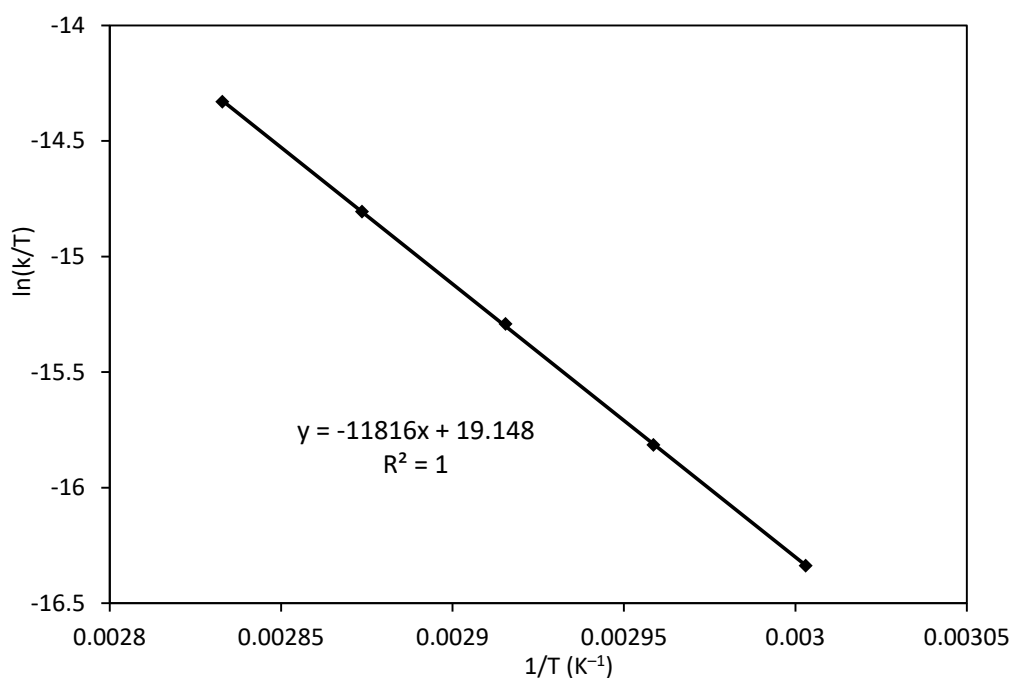


Figure S91. Eyring plot of the conversion of **5** to **3**.

The activation parameters for the conversion of **5** to **3** were determined by measuring rate constants at various temperatures (Fig. S90). An Eyring plot (Fig. S91) was constructed from these data (Table S2), and the activation enthalpy and entropy were extracted as follows: $\Delta H^\ddagger = 23.4(1)$ kcal/mol, $\Delta S^\ddagger = -9.2(3)$ eu, $\Delta G^\ddagger(298\text{K}) = 26.1$ kcal/mol.

4. A formal synthetic cycle for transformation of alkenes and N₂ into alkyl amines

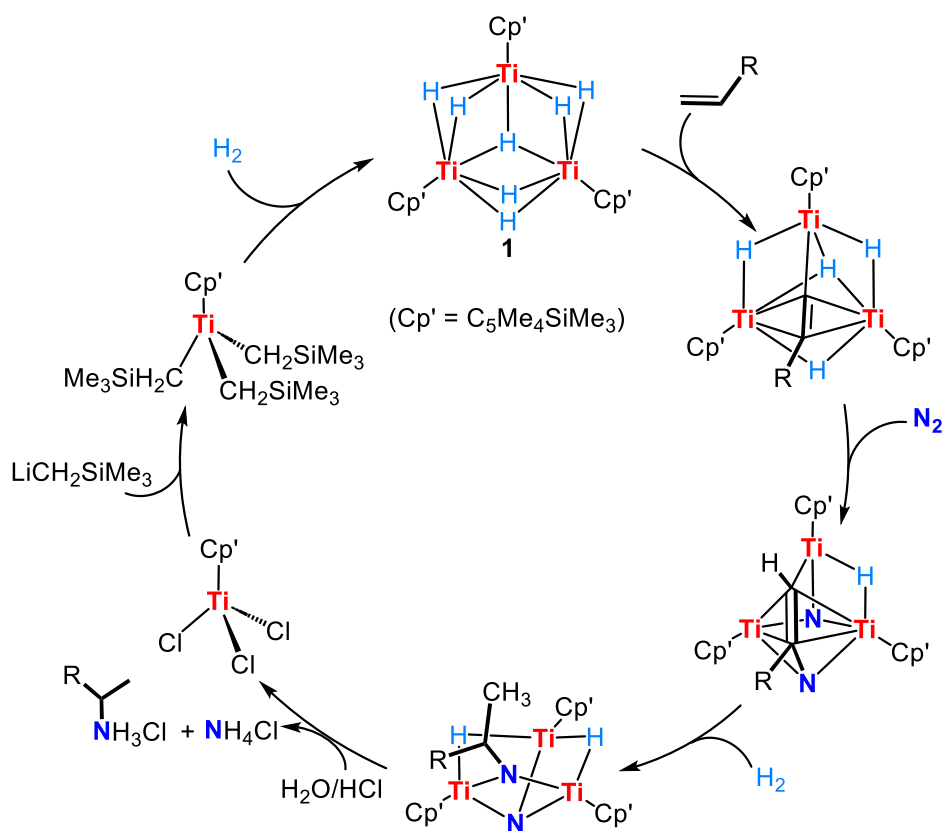


Figure S92. Formal synthetic cycle for transformation of alkenes and N₂ into alkyl amines mediated by titanium complexes. [Cp'TiCl₃] could be easily transformed to [Cp'Ti(CH₂SiMe₃)₃] by reaction with LiCH₂SiMe₃, which could be served as a precursor of the hydride complex **1** by hydrogenolysis with H₂. Thus, a complete synthetic cycle for activation of alkenes, N₂, H₂, and conversion to alkyl amines by using the titanium hydride under ambient conditions could be accomplished.

5. X-ray crystallographic studies

Crystals for X-ray analysis were obtained as described in the preparations. The crystals were manipulated in the glovebox under a microscope in the glovebox, and were mounted on nylon cryoloops with polybutenes ($M_n \sim 920$, Aldrich). Data collections were performed at $-100\text{ }^\circ\text{C}$ on Bruker D8 QUEST diffractometer with CMOS area detector, using an I μ S (Incoatec Microfocus Source) microfocus sealed tube with Mo-K α radiation ($\lambda = 0.71073\text{ \AA}$). The Bravais lattice and the unit cell parameters were determined by the Bruker APEX3 software package⁷. The raw frame data were processed, and absorption corrections were done using SAINT⁷ and SADABS⁷ embedded in Bruker APEX3 to yield the reflection data (hkl) file. All of the structures were solved using SHELXL-2018 (ref. 8). Structural refinement was performed using Olex2 systems⁹, on F^2 anisotropically for all of the non-hydrogen atoms by the full matrix least-squares method. Analytical scattering factors for neutral atoms were used throughout the analysis. Bridging hydride ligands could be located on difference Fourier maps and refined isotropically. Other hydrogen atoms were placed at the calculated positions, which were refined using a riding model. Disorder at the N1, N1A, N1B, and C1, C2, C3, C4, C5, C6 atoms in **3** was refined at 50(N1) :25(N1A) :25(N1B)%, and 75(C1,C3), 50(C2,C5) :25(C4,C6)% occupancy. Disorder at the C16, C17, C18, and C16A, C17A, C18A atoms in **4g** was refined at 52(C16,C17,C18) : 48(C16A,C17A,C18A)% occupancy. Disorder at the C1, C1A, C1B, and N1, N1A, N1B, and C13, C14, C15, C13A, C14A, C15A, and C25, C26, C27, C25A, C26A, C27A, and C37, C38, C39, C37A, C38A, C39A atoms in **6** was refined at 60(C1):20(C1A):20(C1B)%, 40(N1):40(N1A):20(N1B)%, 56(C13,C14,C15): 44(C13A,C14A,C15A)%, 69(C25,C26,C27): 31(C25A,C26A,C27A)%, 50(C37,C38,C39):50(C37A,C38A,C39A)% occupancy. Disorder at the Ti3, Si3, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, and Ti3A, Si3A, C37A, C38A, C39A, C40A, C41A, C42A, C43A, C44A, C45A, C46A, C47A, C48A, C49A, C50A, C51A, atoms in **8g'** was refined at 88(Ti3, Si3, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51) : 12(Ti3A, Si3A, C37A, C38A, C39A, C40A, C41A, C42A, C43A, C44A, C45A, C46A, C47A, C48A, C49A, C50A, C51A)% occupancy.

The analytical scattering factors for neutral atoms were used throughout the analysis. The residual electron densities were of no chemical significance. Crystal data and analysis results are listed in Table S3.

Table S3. X-Ray crystallographic data and structure refinement for **1'**, **3**, **4a**, **4f'**, **4g**, **5**, **6**, **8a**, and **8g'**.

	1'	3	4a	4f'	4g	5	6	8a	8g'
CCDC number	2226119	2184614	2184610	2285950	2226120	2184611	2184612	2184613	2226121
formula	C ₄₅ H ₈₈ Si ₃ Ti ₃ · (C ₆ H ₁₄) _{0.5}	C ₃₉ H ₆₇ N ₂ Si ₃ Ti ₃	C ₃₉ H ₇₀ Si ₃ Ti ₃	C ₅₂ H ₉₄ Si ₃ Ti ₃	C ₄₂ H ₇₄ Si ₃ Ti ₃	C ₃₉ H ₆₈ N ₂ Si ₃ Ti ₃ · (C ₄ H ₁₀ O ₂) _{0.5}	C ₃₉ H ₆₆ N ₂ Si ₃ Ti ₃	C ₃₉ H ₇₂ N ₂ Si ₃ Ti ₃	C ₅₁ H ₉₄ N ₂ Si ₃ Ti ₃
formula weight	900.20	791.91	766.92	947.24	806.98	837.98	792.92	796.95	963.25
crystal system	triclinic	monoclinic	triclinic	triclinic	triclinic	triclinic	monoclinic	triclinic	monoclinic
space group	<i>P</i> -1	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> -1	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> -1	<i>P</i> 2 ₁ / <i>c</i>
a, Å	11.1673(3)	11.5470(2)	10.455(5)	11.8409(7)	10.9833(3)	10.1274(3)	11.4039(6)	11.4141(5)	11.5177(5)
b, Å	11.5091(4)	19.5979(4)	11.285(5)	16.8885(9)	11.4834(3)	11.6114(4)	20.1349(11)	11.9154(5)	40.3561(17)
c, Å	21.5001(7)	19.3634(4)	19.790(9)	28.3739(15)	19.7850(5)	20.2424(6)	19.1121(10)	18.4622(7)	12.1735(5)
α, deg	90.2969(14)		75.297(6)	88.358(3)	75.9095(14)	105.3654(13)		98.606(2)	
β, deg	96.8877(13)	103.0488(8)	76.669(7)	88.355(3)	76.2416(14)	91.3155(12)	90.898(3)	101.647(2)	94.793(2)
γ, deg	96.1696(14)		69.619(6)	79.765(3)	71.6674(15)	92.6611(12)		111.5620(19)	
V, Å ³	2727.02(15)	4268.73(14)	2091.0(16)	5579.9(5)	2261.96(11)	2291.27(13)	4387.9(4)	2217.00(16)	5638.6(4)
Z	2	4	2	4	2	2	4	2	4
D _{calcd} , g/cm ³	1.096	1.232	1.218	1.128	1.185	1.215	1.199	1.194	1.135
temp, K	173(2)	173(2)	173(2)	173(2)	173(2)	173(2)	173(2)	173(2)	173(2)
μ, mm ⁻¹ (MoKα)	0.522	0.660	0.670	0.514	0.622	0.620	0.642	0.635	0.510
2θ _{max}	55.0	50.0	50.0	55.0	60.0	55.0	55.0	55.0	55.0
reflections collected	12420	28221	12004	25351	16061	31944	46018	24279	17749
independent reflections (<i>R</i> _{int})	10633 (0.0465)	7545 (0.0234)	7995 (0.1128)	20335 (0.0404)	9908 (0.0568)	12089 (0.0275)	10048 (0.0754)	6701 (0.0483)	12321 (0.0602)
<i>R</i> 1 (<i>I</i> > 2σ(<i>I</i>))	0.0431	0.0408	0.1076	0.0889	0.0637	0.0483	0.1176	0.0602	0.0737
<i>wR</i> 2 (<i>I</i> > 2σ(<i>I</i>))	0.1132	0.0977	0.2524	0.2173	0.1289	0.1237	0.2857	0.1407	0.1642
<i>wR</i> 2 (all data)	0.1198	0.1000	0.2707	0.2288	0.1509	0.1303	0.2967	0.1527	0.1798
parameters	562	484	440	1131	505	482	532	450	639
GOF	1.016	1.072	0.929	1.053	1.016	1.039	1.123	1.047	1.076

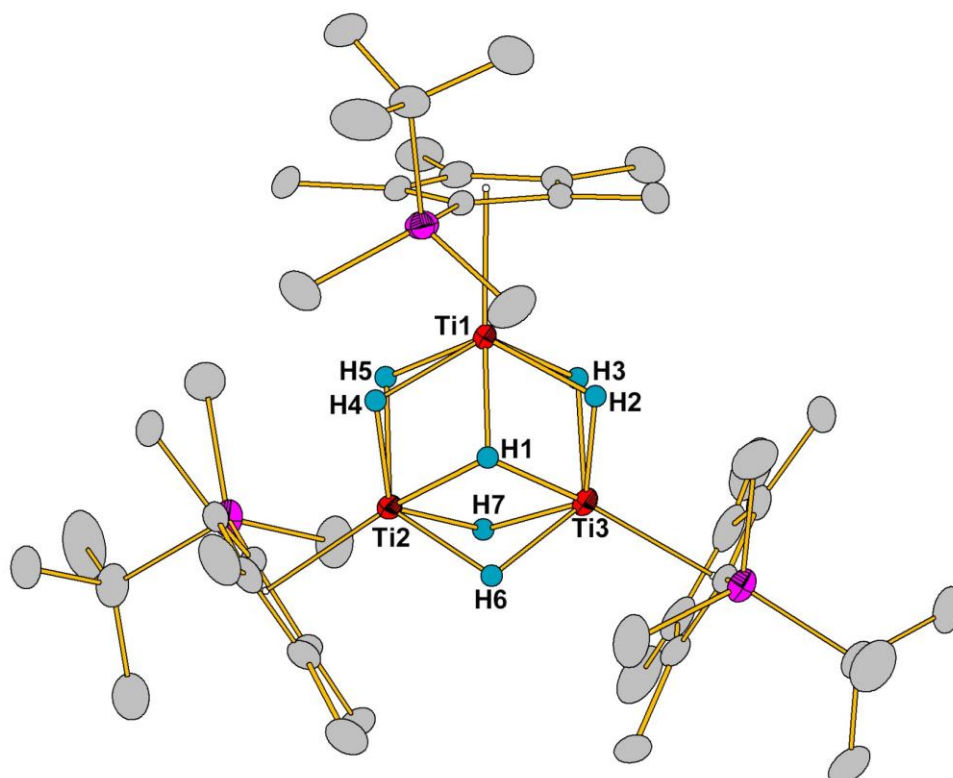


Figure S93. ORTEP drawing of the structure of **1'** with thermal ellipsoids at 30% probability. Co-crystallized hexane was omitted for clarity.

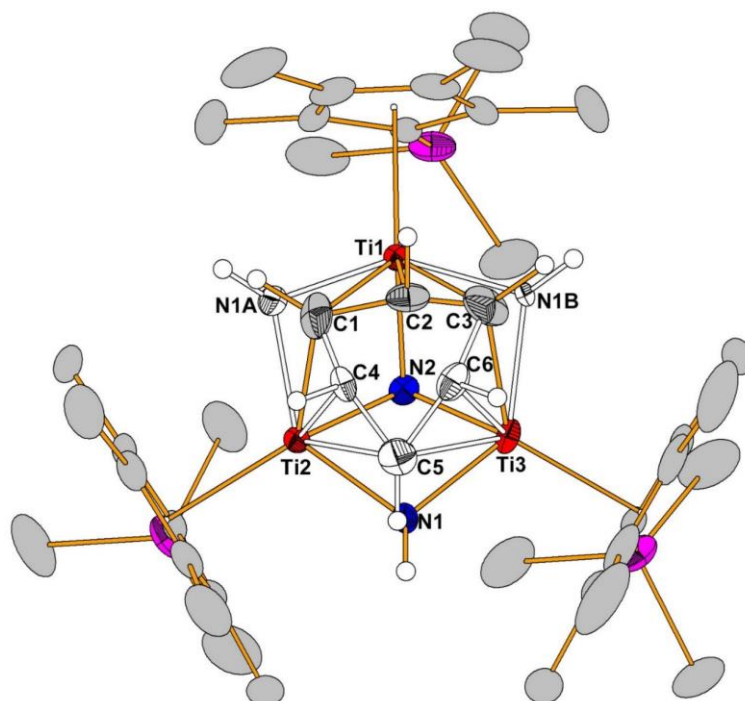


Figure S94. ORTEP drawing of the structure of **3** (N1: N1A: N1B = 50: 25: 25%; C1,C3 : C2,C5 : C4,C6 = 75 : 50 : 25%) with thermal ellipsoids at 30% probability.

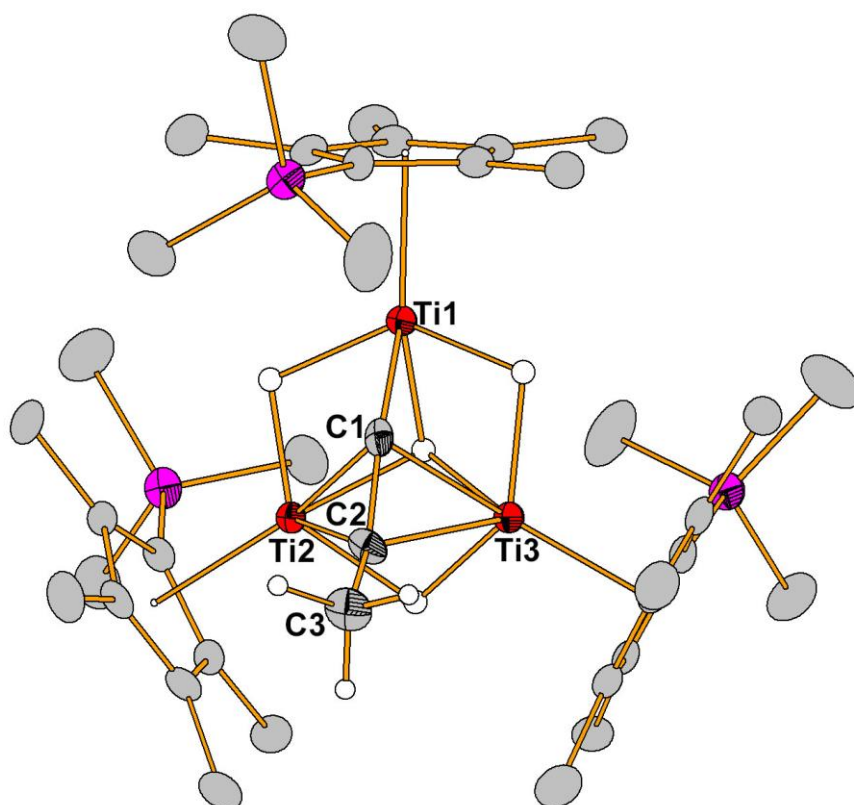


Figure S95. ORTEP drawing of the structure of **4a** with thermal ellipsoids at 30% probability.

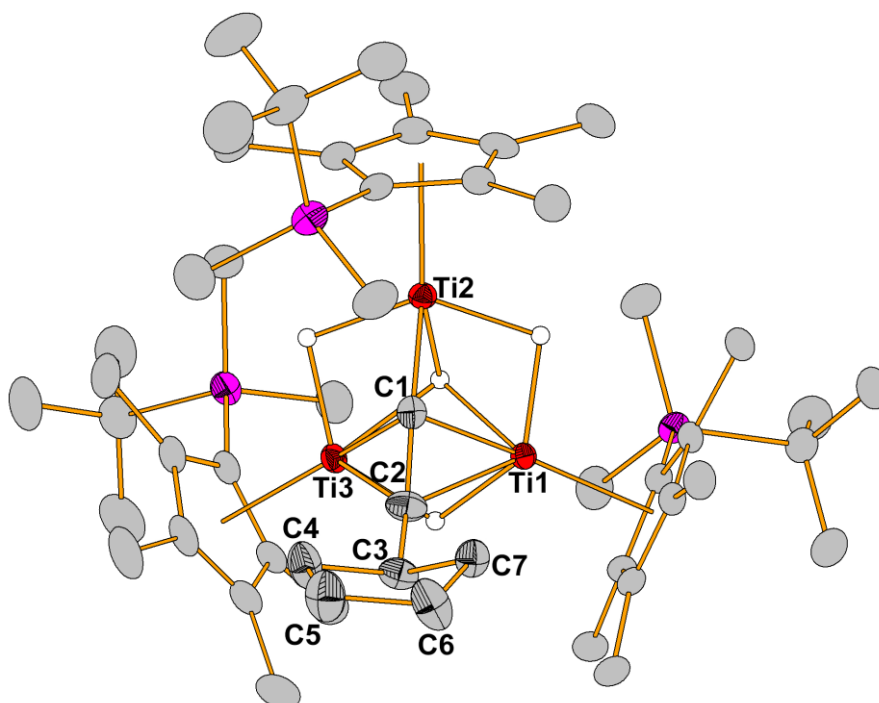


Figure S96. ORTEP drawing of the structure of **4f** with thermal ellipsoids at 30% probability.

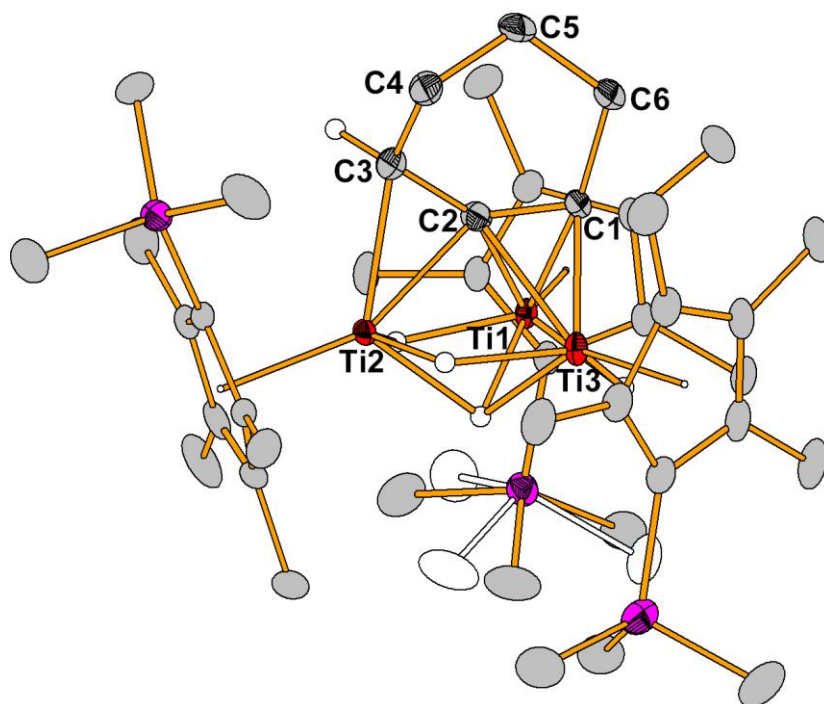


Figure S97. ORTEP drawing of the structure of **4g** with thermal ellipsoids at 30% probability.

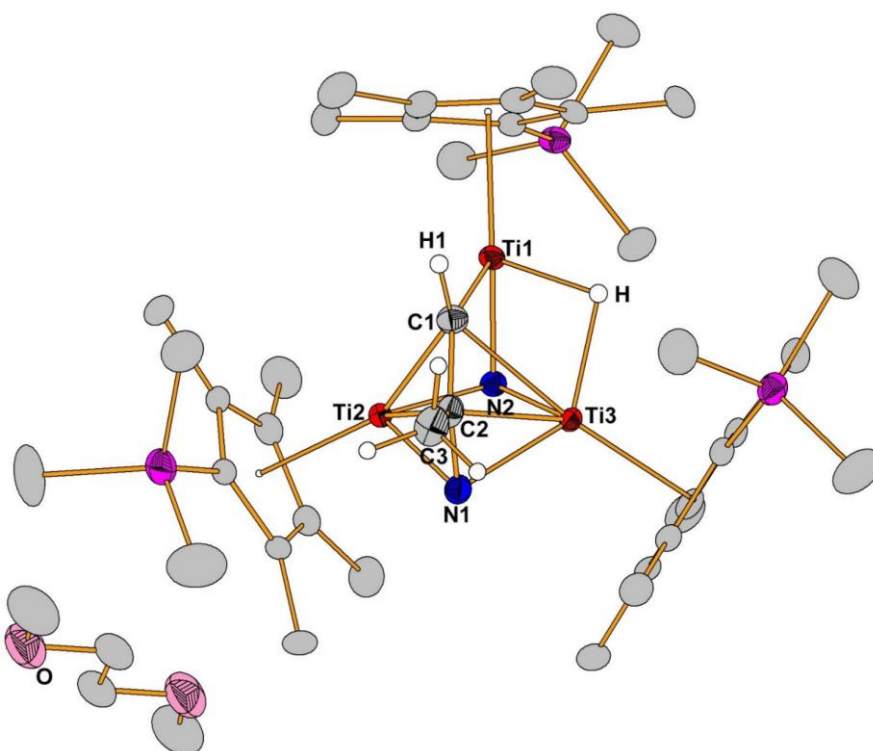


Figure S98. ORTEP drawing of the structures of **5** and co-crystallized DME with thermal ellipsoids at 30% probability.

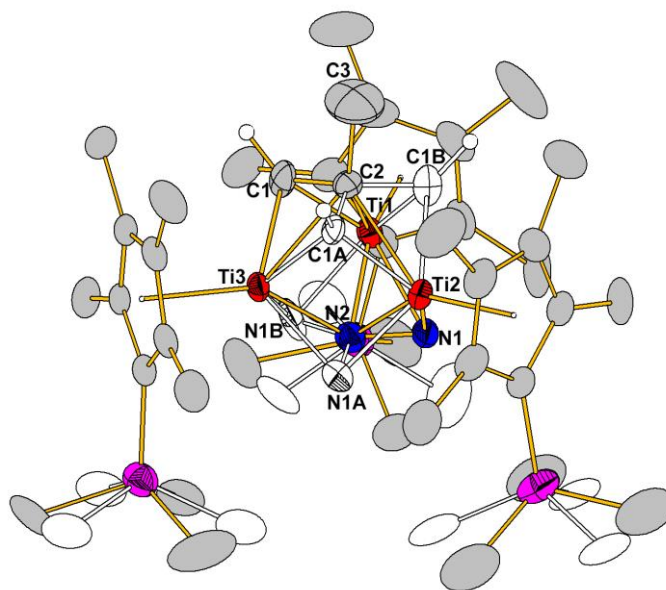


Figure S99. ORTEP drawing of the structure of **6** (C1: C1A: C1B = 60: 20: 20%; N1: N1A: N1B = 40: 40: 20%) with thermal ellipsoids at 25% probability.

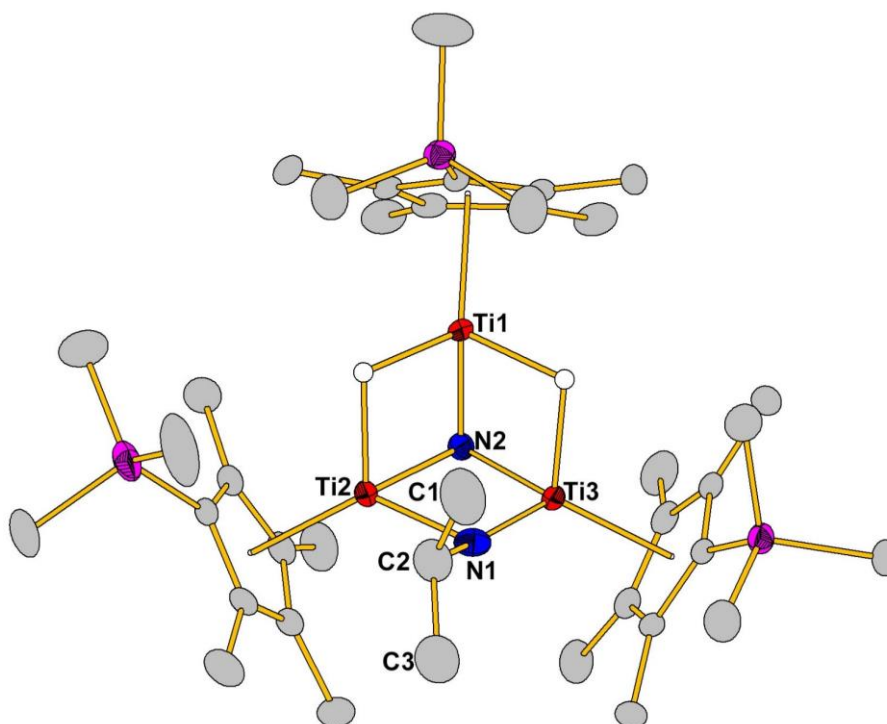


Figure S100. ORTEP drawing of the structure of **8a** with thermal ellipsoids at 30% probability.

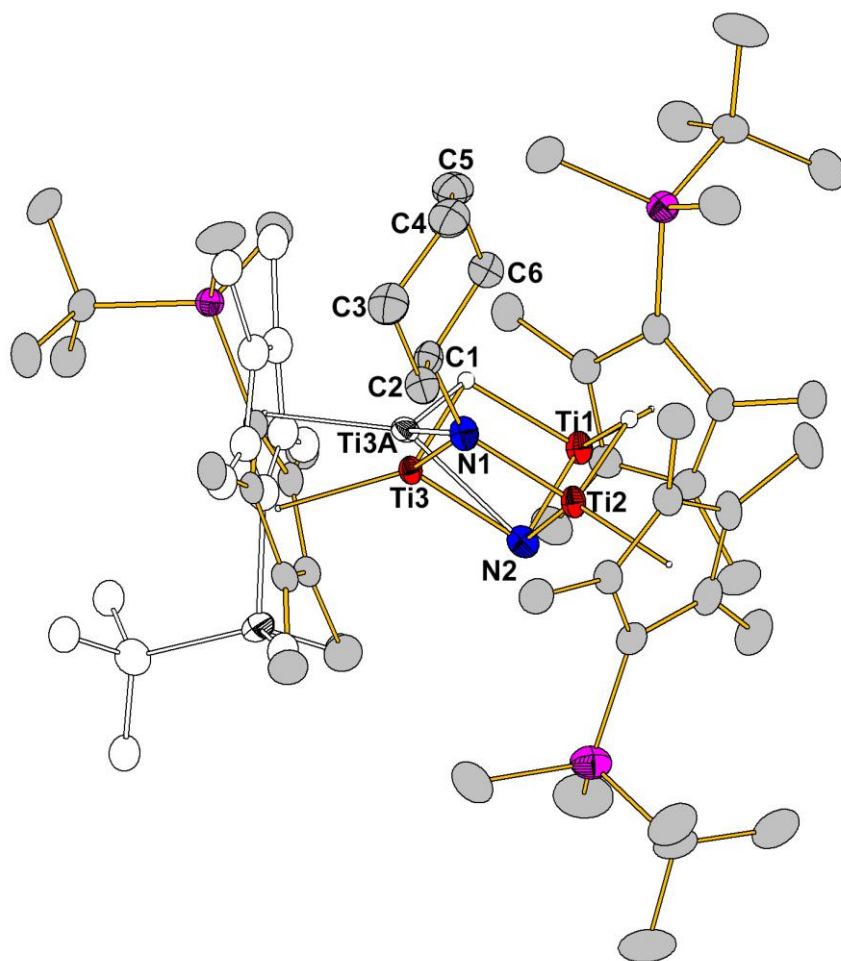


Figure S101. ORTEP drawing of the structure of **8g'** (Ti3 : Ti3A = 88 : 12%) with thermal ellipsoids at 30% probability.

6. DFT calculations

All the DFT calculations were performed using the Gaussian 16 program package¹⁰. The geometries of all stationary points were optimized by unrestricted TPSSSTPSS functional¹¹, which often shows the best performance for the structure and energy calculations for transition-metal-containing systems¹²⁻¹⁴. In the geometrical optimizations, the 6-31G(d) basis set was considered for C, H, N, and Si atoms and the Stuttgart/Dresden^{15,16} effective core potentials (ECP) as well as the associated valence basis sets were used for Ti atoms. Such basis sets are denoted as “BSI”. Considering potential antiferromagnetic coupling in some structures, the combination of the spin-unrestricted manner and the keyword of scf=nosymm was used in optimizations. All structures were optimized without any geometrical symmetry restriction. Frequency calculations of each optimized structure were subsequently analyzed to conform a stationary point as a minimum (no imaginary frequency) or a transition state (one imaginary frequency) and to obtain the thermodynamic corrections to Gibbs free energy. Based on the TPSSSTPSS/BSI geometries optimized in gas-phase, single-point calculations were further performed with higher level basis sets (*i.e.*, BSII) to obtain more accurate energies. In the BSII, the basis sets for Ti atoms are same as that in geometrical optimization, and 6-311+G(d,p) basis sets were utilized for the remaining atoms. In these single-point calculations, the solvation effect of *n*-hexane was also considered by using the SMD¹⁷ solvation model and dispersion corrections were included through GD3BJ approach¹⁸. The stabilities of wave functions were tested by the keyword of stable=opt in this work. The theoretical strategy adopted here has successfully applied in previous similar multinuclear titanium systems^{19,20}. To reduce the overestimation of the entropy contribution derived from the gas-phase model, corrections for free energies were made by -2.6 (or $+2.6$) kcal/mol for two-to-one (or one-to-two) transformations, which have been used in many earlier studies²⁰⁻²³. The relative Gibbs free energies in solution were used for discussion of the mechanism in this study.

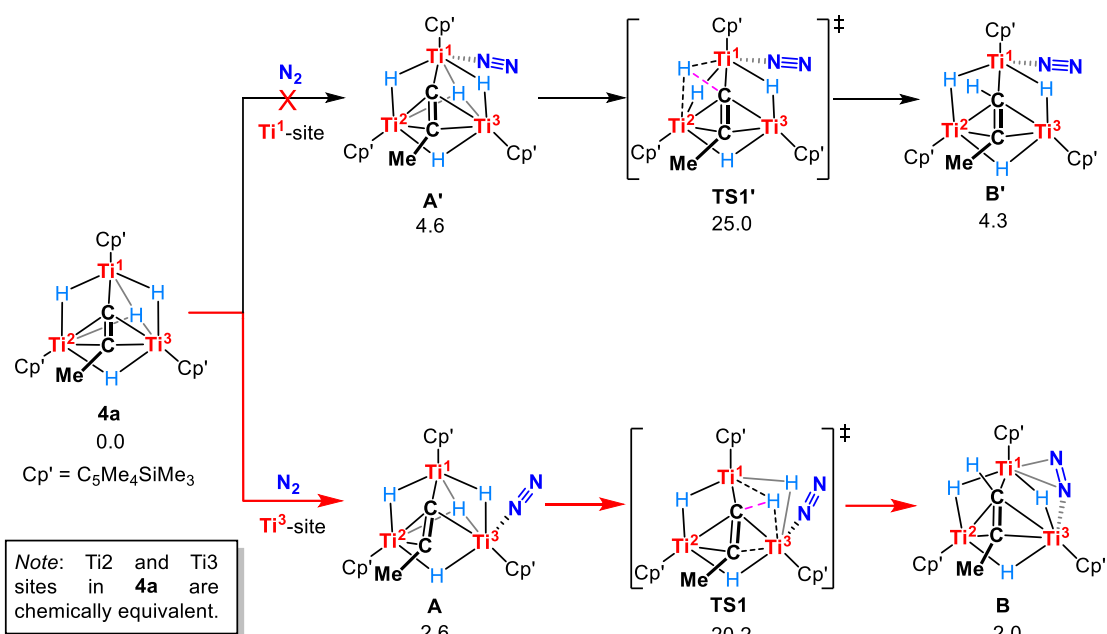


Figure S102. Computed pathways for the initial N_2 coordination and the subsequent reductive elimination of C-H bond. Gibbs free energies are given in kcal/mol.

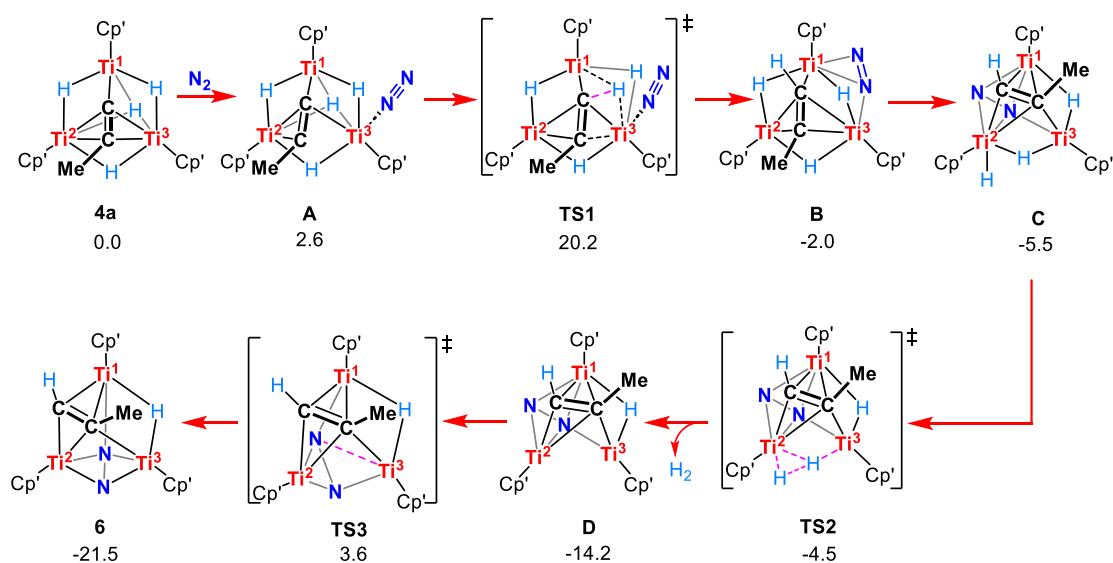


Figure S103. Computed pathway for the conversion of **4a** to **6**. Gibbs free energies are given in kcal/mol.

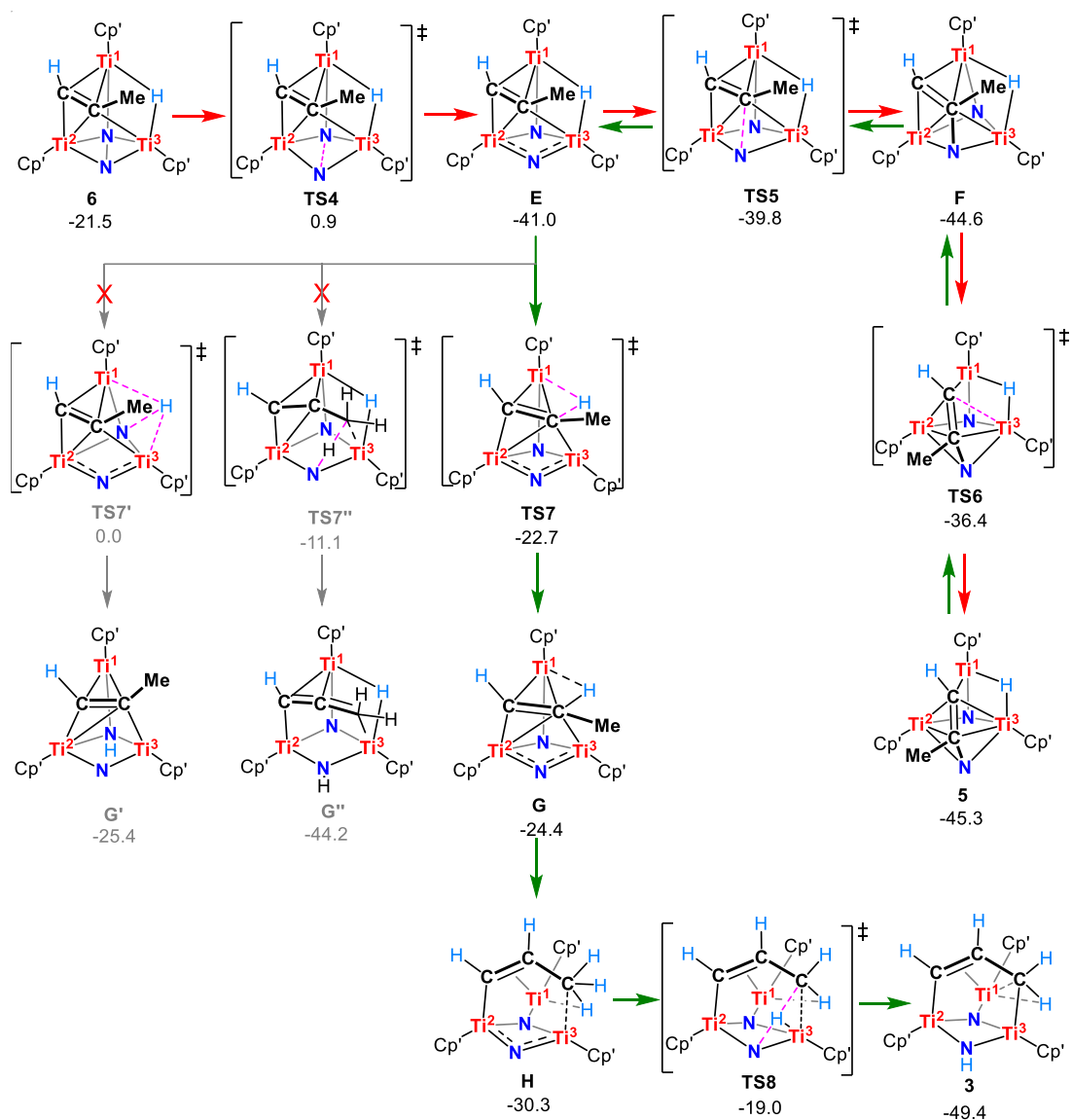


Figure S104. Computed pathways for the conversion of **6** to **5** (red line) and the conversion of **5** to **3** (green line). Gibbs free energies are given in kcal/mol.

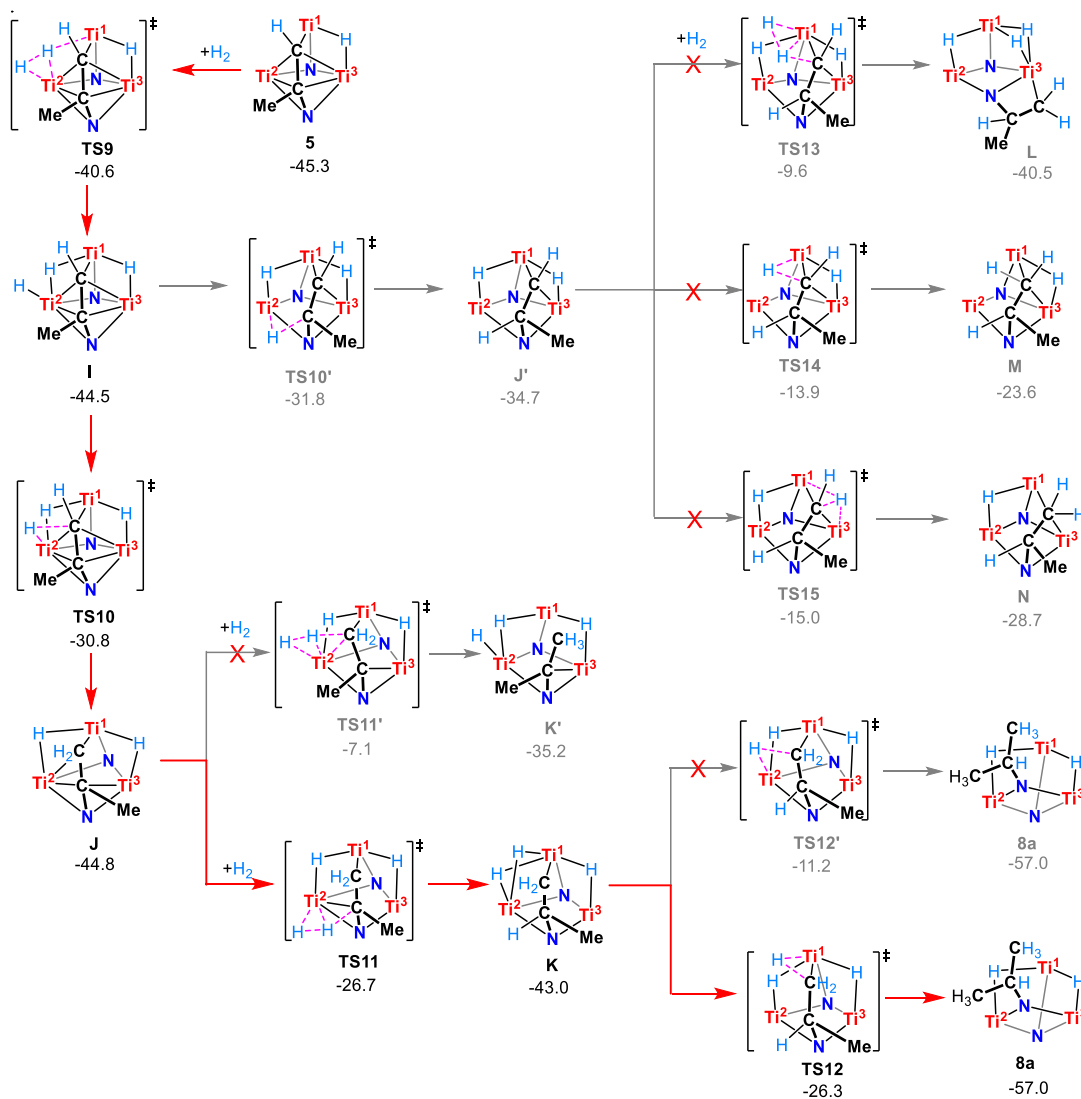


Figure S105. Computed pathways for the conversion of 5 to 8a. The $\text{C}_5\text{Me}_4\text{SiMe}_3$ ligands in displayed structures are omitted for clarity. Gibbs free energies are given in kcal/mol.

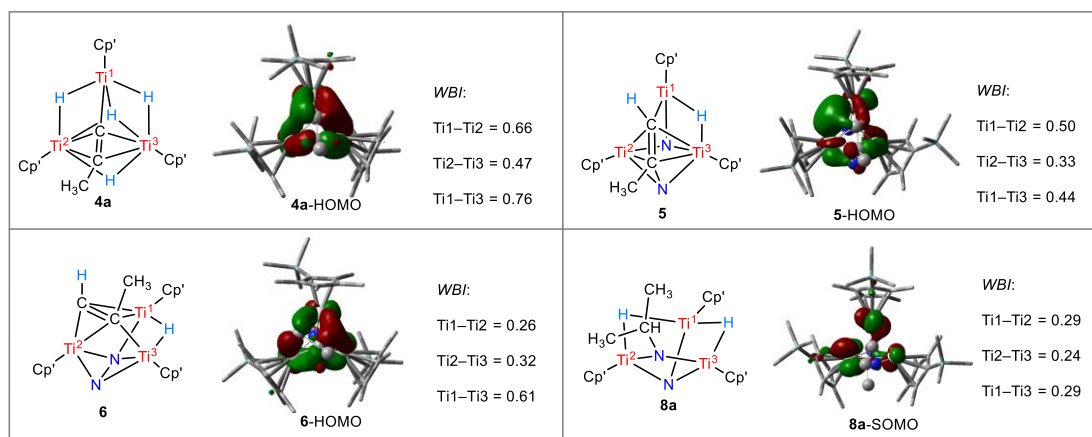


Figure S106. Computational analysis of frontier orbitals (isovalue = 0.04) and Wiberg bond indexes (WBI) of complexes **4a**, **5**, **6**, and **8a** calculated at the level of TPSS-D3BJ (SMD, *n*-hexane)/6-311+G(d,p)-SDD//TPSS/6-31G(d)-SDD. The electron cloud of the singly occupied molecular orbital (SOMO) of complex **8a** is localized on the three Ti centers, with WBI for the Ti–Ti bonds (0.29, 0.24, 0.29). In contrast, the electron cloud of the highest occupied molecular orbitals (HOMO) of complexes **4a**, **5**, and **6** are delocalized between two Ti centers with WBI for Ti–Ti bonds (**4a**, 0.66, 0.47, 0.76; **5**, 0.50, 0.33, 0.44; **6**, 0.26, 0.32, 0.61), suggesting that there are obvious Ti–Ti bonding interactions in complexes **4a**, **5**, and **6**, while weak Ti–Ti bonding interactions in complex **8a**.

Table S4. Imaginary frequency of transition state (cm^{-1}), single-point calculation energy (E_{sp} , a.u.), gas-phase thermal correction to Gibbs free energy ($\Delta\Delta G$, a.u.), relative free energy (ΔG , kcal/mol), and relative free energy corrected by empirical value ($\Delta G_{\text{corr.}}$, kcal/mol).

	Image, Freq.	$\Delta\Delta G$	E_{sp}	$G (\Delta\Delta G + E_{\text{sp}})$	ΔG	$\Delta G_{\text{corr.}}$
N₂	/	-0.013053	-109.570655	-109.583708	/	/
H₂	/	-0.001306	-1.179258	-1.180564	/	/
4a	/	0.864896	-2573.056079	-2572.191183	0.0	0.0
A	/	0.873214	-2682.639760	-2681.766546	5.2	2.6
TS1	-615.61	0.870847	-2682.609434	-2681.738587	22.8	20.2
B	/	0.875591	-2682.649507	-2681.773916	0.6	-2.0
C	/	0.874091	-2682.653628	-2681.779537	-2.9	-5.5
TS2	-627.28	0.873717	-2682.651558	-2681.777841	-1.9	-4.5
D	/	0.859538	-2681.476550	-2680.617012	-14.2	-14.2
TS3	-361.17	0.853239	-2681.441908	-2680.588669	3.6	3.6
6	/	0.858497	-2681.487074	-2680.628577	-21.5	-21.5
TS4	-539.34	0.856910	-2681.449772	-2680.592862	0.9	0.9
E	/	0.856906	-2681.516530	-2680.659624	-41.0	-41.0
TS5	-105.04	0.858309	-2681.516074	-2680.657765	-39.8	-39.8
F	/	0.859309	-2681.524641	-2680.665332	-44.6	-44.6

TS6	-185.36	0.858850	-2681.511209	-2680.652359	-36.4	-36.4
5		0.861132	-2681.527683	-2680.666551	-45.3	-45.3
TS7	-669.65	0.854589	-2681.485116	-2680.630527	-22.7	-22.7
G	/	0.859187	-2681.492434	-2680.633247	-24.4	-24.4
H	/	0.862473	-2681.505099	-2680.642626	-30.3	-30.3
TS8	-1439.92	0.856094	-2681.480671	-2680.624577	-19.0	-19.0
3	/	0.863527	-2681.536627	-2680.673100	-49.4	-49.4
TS9	-579.45	0.872712	-2682.708198	-2681.835486	-38.0	-40.6
I	/	0.873813	-2682.715534	-2681.841721	-41.9	-44.5
TS10	-736.45	0.873811	-2682.693708	-2681.819897	-28.2	-30.8
J		0.876761	-2682.718888	-2681.842127	-42.2	-44.8
TS11	-1101.09	0.893059	-2683.882797	-2682.989738	-21.5	-26.7
K	/	0.899478	-2683.915214	-2683.015736	-37.8	-43.0
TS12	-1025.38	0.896259	-2683.885407	-2682.989148	-21.1	-26.3
8a	/	0.894382	-2683.932322	-2683.037940	-51.8	-57.0
A'	/	0.870780	-2682.634204	-2681.763424	7.2	4.6
TS1'	-692.93	0.867599	-2682.598440	-2681.730841	27.6	25.0
B'	/	0.874859	-2682.638707	-2681.763848	6.9	4.3
TS7''	-1631.49	0.853844	-2681.465871	-2680.612027	-11.1	-11.1
G''	/	0.858645	-2681.523420	-2680.664775	-44.2	-44.2
TS7'	-1140.66	0.853724	-2681.448061	-2680.594337	0.0	0.0
G'	/	0.856935	-2681.491680	-2680.634745	-25.4	-25.4
TS10'	-737.51	0.873143	-2682.694606	-2681.821463	-29.2	-31.8
J'	/	0.877302	-2682.703271	-2681.825969	-32.1	-34.7
TS13	-721.82	0.894352	-2683.856783	-2682.962431	-4.4	-9.6
L	/	0.896801	-2683.908492	-2683.011691	-35.3	-40.5
TS14	-1012.00	0.874476	-2682.667345	-2681.792869	-11.3	-13.9
M	/	0.878277	-2682.686681	-2681.808404	-21.0	-23.6
TS15	-488.24	0.875616	-2682.670331	-2681.794715	-12.4	-15.0
N	/	0.880558	-2682.697070	-2681.816512	-26.1	-28.7
TS11'	-1273.54	0.892475	-2683.850903	-2682.958428	-1.9	-7.1
K'	/	0.895180	-2683.898489	-2683.003309	-30.0	-35.2
TS12'	-686.99	0.893484	-2683.858433	-2682.964949	-6.0	-11.2

7. Optimized Cartesian coordinates for all stationary points

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 N 0.000000000 0.000000000 -0.557023000

H₂
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 H 0.000000000 0.000000000 -0.370085000

Complex 4a
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TS1

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Ti	1.456365000	-0.736727000	-0.698516000
Si	0.277018000	4.576640000	-1.258872000
Si	-4.576617000	-1.274478000	1.488144000
Si	3.995326000	-1.693056000	2.114374000
C	0.186204000	0.853429000	-1.325772000
C	0.553650000	0.028640000	-2.353895000
C	0.486171000	0.159198000	-3.849657000
H	-0.418931000	0.678754000	-4.193423000
H	0.545772000	-0.813985000	-4.355885000
H	1.347000000	0.753229000	-4.195920000
C	0.090550000	3.624753000	0.369659000
C	1.156289000	3.186066000	1.243265000
C	0.579733000	2.630207000	2.434454000
C	-0.842719000	2.736218000	2.330596000
C	-1.150024000	3.336949000	1.068140000
C	-3.528050000	-1.450758000	-0.088580000
C	-3.466725000	-0.565589000	-1.237867000

C	-2.794718000	-1.243956000	-2.302924000
C	-2.403799000	-2.539433000	-1.829929000
C	-2.870175000	-2.678503000	-0.486148000
C	3.426863000	-1.651008000	0.302335000
C	3.816215000	-0.724395000	-0.745136000
C	3.397556000	-1.253911000	-2.008499000
C	2.718305000	-2.488549000	-1.766366000
C	2.743735000	-2.736418000	-0.354724000
H	0.156272000	-2.028552000	-0.834367000
H	1.441967000	0.332218000	0.835353000
H	-1.534029000	0.227043000	0.957179000
H	-1.219286000	0.899110000	-0.908174000
N	-0.700079000	-1.893773000	1.272040000
N	-0.510725000	-2.524233000	2.199003000
C	5.102078000	-3.232212000	2.313951000
H	5.499382000	-3.292134000	3.338903000
H	4.556511000	-4.165635000	2.116701000
H	5.959382000	-3.197922000	1.625474000
C	5.067844000	-0.197877000	2.600034000
H	4.514467000	0.751214000	2.586803000
H	5.421917000	-0.353295000	3.631262000
H	5.955369000	-0.081863000	1.963167000
C	2.579515000	-1.787327000	3.374681000
H	2.987208000	-1.693054000	4.393642000
H	1.859577000	-0.973308000	3.218037000
H	2.020155000	-2.730798000	3.330996000
C	4.645435000	0.531022000	-0.602033000
H	4.420574000	1.070450000	0.321828000
H	5.721872000	0.292126000	-0.596831000
H	4.472048000	1.217182000	-1.441587000
C	3.759146000	-0.688225000	-3.359487000
H	3.700476000	0.407816000	-3.378999000
H	4.792867000	-0.964888000	-3.623207000
H	3.103990000	-1.074269000	-4.148884000
C	2.172652000	-3.421232000	-2.817407000
H	1.810734000	-2.873611000	-3.696957000
H	2.950695000	-4.122534000	-3.161454000
H	1.338781000	-4.017701000	-2.429008000
C	2.202275000	-3.987786000	0.296951000
H	2.935418000	-4.807957000	0.232709000
H	1.970706000	-3.828991000	1.355843000
H	1.281948000	-4.329528000	-0.194649000
C	2.638031000	3.384994000	1.029686000
H	2.951187000	3.123460000	0.014713000
H	2.916961000	4.436904000	1.206748000
H	3.220703000	2.772632000	1.728191000
C	1.332132000	2.117306000	3.638486000
H	2.295911000	1.676259000	3.359582000
H	1.533010000	2.934537000	4.350393000
H	0.761081000	1.349206000	4.175832000
C	-1.827851000	2.348533000	3.406652000
H	-1.464566000	1.499990000	4.000487000
H	-1.994119000	3.187776000	4.101445000
H	-2.801268000	2.066609000	2.989065000
C	-2.541064000	3.728374000	0.623775000
H	-2.695806000	4.812326000	0.750089000
H	-2.726939000	3.488545000	-0.427895000
H	-3.305761000	3.220208000	1.223781000
C	-1.163760000	4.276888000	-2.466430000
H	-1.361468000	3.203280000	-2.592342000
H	-2.096031000	4.769178000	-2.157806000
H	-0.892024000	4.683807000	-3.452986000
C	1.871459000	4.136646000	-2.199877000
H	2.776003000	4.545420000	-1.729380000
H	1.990240000	3.048362000	-2.295695000
H	1.813156000	4.558220000	-3.215576000
C	0.324866000	6.437368000	-0.845443000

H	1.168840000	6.679870000	-0.182776000
H	0.432160000	7.045135000	-1.756964000
H	-0.595542000	6.760737000	-0.336915000
C	-4.137077000	0.779081000	-1.394128000
H	-5.196469000	0.656061000	-1.674112000
H	-4.099767000	1.363752000	-0.471739000
H	-3.656412000	1.369650000	-2.184091000
C	-2.788363000	-3.960381000	0.308500000
H	-2.884262000	-3.782926000	1.385092000
H	-3.594989000	-4.647641000	0.008145000
H	-1.835269000	-4.480321000	0.143706000
C	-1.752581000	-3.617823000	-2.659475000
H	-1.207002000	-4.332471000	-2.031476000
H	-2.512027000	-4.184095000	-3.223257000
H	-1.043375000	-3.198344000	-3.382957000
C	-2.730471000	-0.780137000	-3.735312000
H	-1.912851000	-1.259326000	-4.284883000
H	-3.670099000	-1.037459000	-4.251644000
H	-2.604094000	0.306409000	-3.815653000
C	-5.470734000	0.399658000	1.614080000
H	-4.778616000	1.246973000	1.712397000
H	-6.133035000	0.598835000	0.760811000
H	-6.097497000	0.383831000	2.519474000
C	-3.609217000	-1.492748000	3.108013000
H	-3.162436000	-2.489066000	3.223369000
H	-2.798178000	-0.756439000	3.186251000
H	-4.291990000	-1.337324000	3.958203000
C	-5.937794000	-2.606215000	1.403928000
H	-6.611899000	-2.521645000	2.270131000
H	-6.547866000	-2.494731000	0.495322000
H	-5.527733000	-3.625768000	1.404131000

B

Ti	0.597380000	1.111507000	-0.780073000
Ti	0.712260000	-1.191216000	0.614630000
Ti	-1.700992000	0.174090000	0.695895000
Si	2.912924000	3.617234000	1.100459000
Si	2.537049000	-3.638683000	-1.696759000
Si	-4.369705000	-0.414276000	-1.903804000
C	0.168871000	0.953646000	1.357079000
C	-0.424850000	-0.009378000	2.217702000
C	-0.278457000	0.002194000	3.723720000
H	0.773008000	0.083042000	4.037744000
H	-0.708905000	-0.886308000	4.199582000
H	-0.799202000	0.878995000	4.143684000
C	1.925668000	3.045833000	-0.414645000
C	0.628482000	3.494403000	-0.855299000
C	0.409595000	3.028442000	-2.195628000
C	1.576878000	2.314383000	-2.615964000
C	2.498199000	2.301541000	-1.526127000
C	2.007428000	-3.057453000	0.031464000
C	2.799754000	-2.285258000	0.957710000
C	2.159163000	-2.284463000	2.239528000
C	0.953784000	-3.050171000	2.128331000
C	0.849673000	-3.512152000	0.773907000
C	-3.892646000	0.038851000	-0.123320000
C	-3.759852000	1.343624000	0.490829000
C	-3.534918000	1.177591000	1.891887000
C	-3.538088000	-0.227439000	2.180376000
C	-3.755944000	-0.925345000	0.950243000
H	-1.100196000	-1.532350000	0.320170000
H	0.815203000	1.726617000	1.788089000
H	-1.256293000	1.116885000	-0.832927000
H	1.917998000	0.108778000	0.070678000
N	0.367089000	-0.899184000	-1.316490000
N	0.285732000	-0.347815000	-2.375167000
C	-6.083648000	-1.246469000	-1.844487000

H	-6.420431000	-1.511210000	-2.858611000
H	-6.078139000	-2.168976000	-1.246979000
H	-6.837051000	-0.574215000	-1.407753000
C	-4.521791000	1.094942000	-3.049631000
H	-3.560233000	1.605683000	-3.195788000
H	-4.859157000	0.744474000	-4.037648000
H	-5.254124000	1.833757000	-2.696472000
C	-3.129541000	-1.597841000	-2.721704000
H	-3.477591000	-1.850510000	-3.735957000
H	-2.138684000	-1.132086000	-2.814816000
H	-3.000545000	-2.542265000	-2.175121000
C	-3.913413000	2.684490000	-0.186728000
H	-3.431378000	2.705957000	-1.168431000
H	-4.979760000	2.921704000	-0.331009000
H	-3.481446000	3.487723000	0.422469000
C	-3.394529000	2.284555000	2.909036000
H	-2.902397000	3.169670000	2.485923000
H	-4.382209000	2.602535000	3.280026000
H	-2.807340000	1.961744000	3.777745000
C	-3.524045000	-0.860698000	3.548359000
H	-3.090603000	-0.194946000	4.302943000
H	-4.552425000	-1.096946000	3.867412000
H	-2.954614000	-1.798564000	3.559920000
C	-3.950856000	-2.421691000	0.856054000
H	-4.998033000	-2.687853000	1.074130000
H	-3.709277000	-2.805173000	-0.140817000
H	-3.319118000	-2.954249000	1.578085000
C	1.850032000	4.484676000	2.420575000
H	2.511372000	4.786381000	3.248021000
H	1.360394000	5.393184000	2.045244000
H	1.073760000	3.832623000	2.845812000
C	4.203278000	4.881475000	0.496925000
H	4.812010000	5.251492000	1.336123000
H	4.889012000	4.442430000	-0.241884000
H	3.720920000	5.749978000	0.025057000
C	3.822215000	2.192790000	1.979827000
H	4.085576000	2.495665000	3.005088000
H	3.188561000	1.297418000	2.038796000
H	4.755722000	1.910937000	1.473136000
C	3.903104000	1.749232000	-1.601437000
H	4.599160000	2.516082000	-1.979287000
H	4.263123000	1.420552000	-0.621226000
H	3.964800000	0.892018000	-2.283175000
C	1.811067000	1.751608000	-3.995094000
H	2.262867000	2.515806000	-4.648207000
H	2.490082000	0.890506000	-3.974392000
H	0.874741000	1.420410000	-4.459033000
C	-0.783105000	3.311042000	-3.075326000
H	-0.573931000	4.153436000	-3.754673000
H	-1.035926000	2.441546000	-3.695522000
H	-1.669866000	3.572929000	-2.487283000
C	-0.337723000	4.363265000	-0.085015000
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H	-0.010374000	5.415417000	-0.093875000
H	-1.337858000	4.327773000	-0.531089000
C	3.531243000	-2.336374000	-2.663633000
H	4.544959000	-2.185486000	-2.268644000
H	3.634195000	-2.672222000	-3.707193000
H	3.015531000	-1.367194000	-2.679123000
C	3.649201000	-5.166014000	-1.443432000
H	3.110020000	-5.973938000	-0.927083000
H	4.001422000	-5.563441000	-2.407636000
H	4.536262000	-4.923867000	-0.839546000
C	1.079822000	-4.144718000	-2.806617000
H	0.334205000	-3.344091000	-2.902719000
H	1.468629000	-4.356200000	-3.815088000
H	0.570424000	-5.052876000	-2.457601000

C	4.168327000	-1.695233000	0.706485000
H	4.942990000	-2.475468000	0.790514000
H	4.246648000	-1.248578000	-0.288855000
H	4.405293000	-0.917053000	1.441879000
C	2.769952000	-1.731470000	3.505485000
H	3.659800000	-2.317501000	3.785473000
H	3.091897000	-0.687194000	3.395572000
H	2.069720000	-1.778065000	4.346951000
C	0.027076000	-3.456640000	3.247771000
H	0.120026000	-4.535923000	3.448175000
H	0.262188000	-2.928887000	4.178627000
H	-1.023878000	-3.254578000	3.003828000
C	-0.248182000	-4.428157000	0.279301000
H	-0.632201000	-4.119845000	-0.698354000
H	0.117640000	-5.464092000	0.188755000
H	-1.091704000	-4.436722000	0.979947000

C			
Ti	0.992989000	0.943076000	-0.568329000
Ti	0.520839000	-1.401909000	0.658567000
Ti	-1.665667000	0.465455000	0.619238000
Si	4.204042000	2.680080000	0.583582000
Si	0.861959000	-4.320852000	-1.709103000
Si	-4.700083000	0.530260000	-1.481473000
C	0.244577000	1.719494000	1.160930000
C	0.655733000	0.545059000	1.760698000
C	1.057517000	0.499596000	3.231899000
H	0.769420000	1.421770000	3.763301000
H	2.149315000	0.392858000	3.310392000
H	0.608784000	-0.355835000	3.751688000
C	2.907236000	2.343814000	-0.756259000
C	1.758551000	3.155930000	-1.116670000
C	1.163912000	2.606761000	-2.292888000
C	1.931591000	1.457103000	-2.682411000
C	3.013490000	1.311845000	-1.763965000
C	0.946974000	-3.633897000	0.062236000
C	2.095310000	-3.174128000	0.817258000
C	1.690446000	-2.917727000	2.169027000
C	0.288264000	-3.200447000	2.269173000
C	-0.166217000	-3.642441000	0.985885000
C	-3.837475000	1.160351000	0.091413000
C	-3.082994000	2.372674000	0.301976000
C	-2.672653000	2.419380000	1.670313000
C	-3.158188000	1.235937000	2.324626000
C	-3.906887000	0.482608000	1.370657000
H	-0.886898000	-0.825187000	1.730898000
H	0.171320000	2.674518000	1.690474000
H	-2.351009000	-1.093047000	0.834692000
H	1.981932000	-0.592008000	-0.116648000
N	-0.393639000	-0.527531000	-0.673723000
N	-0.899668000	0.585884000	-1.268121000
C	-4.398933000	1.626421000	-3.003779000
H	-4.973308000	1.212657000	-3.847587000
H	-4.725037000	2.666007000	-2.863334000
H	-3.340310000	1.630863000	-3.297593000
C	-6.578185000	0.526971000	-1.152888000
H	-7.123804000	0.184727000	-2.045732000
H	-6.858610000	-0.133536000	-0.320598000
H	-6.939441000	1.537256000	-0.909570000
C	-4.132666000	-1.220270000	-1.954567000
H	-4.675431000	-1.557171000	-2.852126000
H	-3.058624000	-1.220121000	-2.184468000
H	-4.300753000	-1.963242000	-1.163285000
C	-4.760763000	-0.714151000	1.717816000
H	-5.747496000	-0.382211000	2.080693000
H	-4.920858000	-1.366599000	0.853088000
H	-4.299966000	-1.318380000	2.509391000

C	-3.008284000	0.912208000	3.792522000
H	-3.836766000	1.340055000	4.380630000
H	-3.006695000	-0.171480000	3.966050000
H	-2.073499000	1.315910000	4.203168000
C	-2.063910000	3.603133000	2.379605000
H	-2.863302000	4.242550000	2.788660000
H	-1.429854000	3.298546000	3.222626000
H	-1.460187000	4.225530000	1.708015000
C	-2.837018000	3.472555000	-0.698607000
H	-2.593626000	3.072909000	-1.686229000
H	-3.727768000	4.113201000	-0.802821000
H	-2.006788000	4.115018000	-0.381005000
C	3.581673000	3.835513000	1.960316000
H	4.364022000	3.914163000	2.731393000
H	3.370772000	4.852721000	1.604235000
H	2.675856000	3.449772000	2.449144000
C	4.793374000	1.078815000	1.437622000
H	5.594342000	0.574259000	0.879144000
H	5.193230000	1.316352000	2.435575000
H	3.968471000	0.363825000	1.564262000
C	5.706292000	3.510718000	-0.241782000
H	6.499784000	3.714484000	0.493462000
H	6.137342000	2.873440000	-1.027716000
H	5.429230000	4.467425000	-0.708305000
C	4.125489000	0.298021000	-1.901793000
H	4.988095000	0.746827000	-2.420817000
H	4.469801000	-0.072120000	-0.931460000
H	3.805144000	-0.568945000	-2.492874000
C	1.633081000	0.604240000	-3.891932000
H	1.984040000	1.095822000	-4.813778000
H	2.124907000	-0.374738000	-3.834334000
H	0.553330000	0.434078000	-3.996974000
C	0.005303000	3.143460000	-3.091756000
H	0.350088000	3.502239000	-4.074544000
H	-0.747586000	2.361750000	-3.262088000
H	-0.486211000	3.982238000	-2.587070000
C	1.329717000	4.445871000	-0.460064000
H	1.283281000	4.362808000	0.631361000
H	2.034041000	5.257865000	-0.700946000
H	0.339625000	4.757073000	-0.813950000
C	2.621862000	-2.592386000	3.312830000
H	3.378662000	-1.847140000	3.034883000
H	2.077937000	-2.207756000	4.183733000
H	3.160388000	-3.497445000	3.637230000
C	-0.551874000	-3.174676000	3.522757000
H	-0.572464000	-4.170828000	3.994001000
H	-0.159925000	-2.469785000	4.267195000
H	-1.587574000	-2.888689000	3.301326000
C	-1.580339000	-4.098847000	0.709906000
H	-1.767181000	-4.214283000	-0.362793000
H	-1.771818000	-5.071444000	1.191380000
H	-2.315775000	-3.379624000	1.094911000
C	3.532158000	-3.097194000	0.352814000
H	4.019104000	-4.082395000	0.439044000
H	3.614357000	-2.772350000	-0.687700000
H	4.106505000	-2.393228000	0.967802000
C	2.520152000	-4.208615000	-2.635095000
H	3.337845000	-4.733933000	-2.123218000
H	2.394597000	-4.679316000	-3.622777000
H	2.836842000	-3.170294000	-2.808969000
C	0.417270000	-6.168691000	-1.578709000
H	-0.553427000	-6.328309000	-1.088549000
H	0.364382000	-6.627519000	-2.577861000
H	1.174017000	-6.717488000	-0.998835000
C	-0.421455000	-3.437375000	-2.796002000
H	-1.445892000	-3.507727000	-2.406986000
H	-0.186622000	-2.368753000	-2.892447000

H	-0.418338000	-3.881382000	-3.804169000
TS2			
Ti	-0.629106000	1.139361000	0.531173000
Ti	-0.681889000	-1.381399000	-0.417453000
Ti	1.850877000	-0.005174000	-0.495765000
Si	-3.173338000	3.543849000	-1.052144000
Si	-3.638776000	-3.081685000	1.274789000
Si	4.748379000	-0.708500000	1.654073000
C	0.338232000	1.484719000	-1.237860000
C	-0.309439000	0.350736000	-1.720421000
C	-0.726037000	0.259511000	-3.190176000
H	-0.612336000	1.229881000	-3.701020000
H	-1.773949000	-0.056660000	-3.290451000
H	-0.112159000	-0.477499000	-3.723751000
C	-2.083065000	3.030808000	0.411312000
C	-0.770831000	3.532974000	0.776421000
C	-0.414943000	2.993377000	2.049494000
C	-1.493237000	2.156713000	2.493614000
C	-2.525067000	2.201427000	1.509216000
C	-2.256665000	-3.082349000	-0.022596000
C	-2.350909000	-2.805942000	-1.447671000
C	-1.118463000	-3.165629000	-2.064082000
C	-0.239356000	-3.674574000	-1.042523000
C	-0.939889000	-3.642567000	0.199266000
C	4.123655000	0.109600000	0.056067000
C	3.709508000	1.474191000	-0.170188000
C	3.330598000	1.612832000	-1.540613000
C	3.510626000	0.339337000	-2.185127000
C	4.034595000	-0.571670000	-1.219315000
H	0.999755000	-1.387794000	-1.364336000
H	0.585908000	2.348190000	-1.863730000
H	2.101054000	-1.698089000	-0.740174000
H	-1.947503000	-0.177220000	0.195605000
N	0.387231000	-0.593039000	0.858654000
N	1.110244000	0.444653000	1.357479000
C	4.682558000	0.439520000	3.165421000
H	5.089631000	-0.102941000	4.033217000
H	5.275734000	1.355822000	3.042734000
H	3.649450000	0.723913000	3.408084000
C	6.568657000	-1.209476000	1.390339000
H	6.975203000	-1.677639000	2.299973000
H	6.691933000	-1.925846000	0.566007000
H	7.191371000	-0.331929000	1.161415000
C	3.728117000	-2.249240000	2.106387000
H	4.123451000	-2.697386000	3.031908000
H	2.679020000	-1.974079000	2.282996000
H	3.742915000	-3.025717000	1.329107000
C	4.560647000	-1.950425000	-1.544441000
H	5.607032000	-1.884559000	-1.884865000
H	4.531860000	-2.615288000	-0.674511000
H	3.980915000	-2.425985000	-2.345721000
C	3.301409000	0.060278000	-3.654973000
H	4.196043000	0.325632000	-4.241891000
H	3.094399000	-1.002153000	-3.837677000
H	2.461127000	0.637981000	-4.062668000
C	3.041988000	2.906757000	-2.258908000
H	3.984367000	3.364669000	-2.601701000
H	2.416549000	2.750383000	-3.147539000
H	2.537197000	3.636508000	-1.614956000
C	3.759586000	2.608612000	0.820234000
H	3.345430000	2.319708000	1.789842000
H	4.798028000	2.940357000	0.980414000
H	3.193426000	3.473522000	0.454471000
C	-2.204768000	4.382436000	-2.458544000
H	-2.902162000	4.590933000	-3.284987000
H	-1.755832000	5.339305000	-2.160490000

H	-1.407081000	3.739620000	-2.857193000
C	-4.093780000	2.065645000	-1.830682000
H	-5.026390000	1.822166000	-1.302280000
H	-4.364359000	2.304582000	-2.870838000
H	-3.468043000	1.163017000	-1.844760000
C	-4.463991000	4.791765000	-0.415120000
H	-5.134516000	5.115751000	-1.225811000
H	-5.088806000	4.356722000	0.378532000
H	-3.982465000	5.689645000	-0.000741000
C	-3.888973000	1.572699000	1.667138000
H	-4.577707000	2.279140000	2.158865000
H	-4.325454000	1.297186000	0.702258000
H	-3.850517000	0.667834000	2.284889000
C	-1.513529000	1.435172000	3.819617000
H	-1.659020000	2.149373000	4.646399000
H	-2.324865000	0.700070000	3.873961000
H	-0.565555000	0.910457000	4.002013000
C	0.798682000	3.295219000	2.888595000
H	0.505782000	3.835319000	3.803071000
H	1.306459000	2.369079000	3.190829000
H	1.522408000	3.919238000	2.353568000
C	0.032869000	4.571576000	0.033183000
H	0.083293000	4.369863000	-1.042026000
H	-0.411510000	5.571493000	0.161547000
H	1.060166000	4.619760000	0.413627000
C	-0.804902000	-3.186420000	-3.540314000
H	-1.467316000	-2.528619000	-4.114616000
H	0.230486000	-2.880032000	-3.741136000
H	-0.926961000	-4.206056000	-3.939910000
C	1.120274000	-4.282472000	-1.278202000
H	1.039375000	-5.375441000	-1.394338000
H	1.587677000	-3.884164000	-2.187051000
H	1.804953000	-4.084324000	-0.443853000
C	-0.387929000	-4.183793000	1.499264000
H	-0.794961000	-3.657863000	2.369102000
H	-0.631703000	-5.253273000	1.607982000
H	0.704458000	-4.089695000	1.538385000
C	-3.566719000	-2.291875000	-2.185191000
H	-4.332038000	-3.078907000	-2.275289000
H	-4.030117000	-1.438695000	-1.677304000
H	-3.308610000	-1.975685000	-3.203697000
C	-5.189710000	-2.135279000	0.717201000
H	-5.670715000	-2.587738000	-0.160565000
H	-5.923858000	-2.152185000	1.537877000
H	-4.978228000	-1.082865000	0.486473000
C	-4.149740000	-4.893105000	1.569996000
H	-3.304324000	-5.500566000	1.924219000
H	-4.946161000	-4.959116000	2.327126000
H	-4.527124000	-5.358145000	0.647374000
C	-3.072676000	-2.335815000	2.934685000
H	-2.547468000	-3.064585000	3.568008000
H	-2.401760000	-1.479757000	2.780764000
H	-3.947030000	-1.984201000	3.504240000

D

Ti	-1.362134000	1.034065000	-0.534616000
Ti	-0.327853000	-1.418880000	-0.834005000
Ti	1.433006000	0.886933000	-0.480670000
Si	-3.433041000	1.620871000	2.521572000
Si	-0.485343000	-4.163847000	1.788648000
Si	4.135036000	0.535305000	2.122812000
N	0.010717000	-0.173694000	0.488629000
N	0.047835000	1.130118000	0.944905000
C	0.109995000	1.516510000	-1.907861000
H	0.214040000	2.302521000	-2.665056000
C	0.088983000	0.111481000	-2.247561000
C	0.064157000	-0.187464000	-3.753470000

H	-0.969653000	-0.145298000	-4.131340000
H	0.464299000	-1.174394000	-4.005600000
H	0.644865000	0.564376000	-4.314764000
C	-3.107128000	2.025331000	0.695090000
C	-2.307229000	3.091667000	0.132920000
C	-2.416846000	3.042879000	-1.295927000
C	-3.277183000	1.944951000	-1.635256000
C	-3.716109000	1.336798000	-0.419928000
C	-0.413575000	-3.630359000	-0.032736000
C	-1.491003000	-3.466447000	-0.983648000
C	-0.929004000	-3.288460000	-2.295550000
C	0.495706000	-3.333328000	-2.174550000
C	0.814760000	-3.519496000	-0.793453000
C	3.469769000	1.292851000	0.514576000
C	3.763769000	0.927396000	-0.860759000
C	3.247491000	1.938490000	-1.722100000
C	2.647476000	2.958662000	-0.906989000
C	2.782700000	2.573855000	0.460154000
H	-2.003759000	-0.711762000	-0.865596000
C	-5.276973000	1.951779000	2.871722000
H	-5.934735000	1.332501000	2.245179000
H	-5.519052000	1.734046000	3.923281000
H	-5.534579000	3.004174000	2.681439000
C	-2.408769000	2.677150000	3.721471000
H	-2.682810000	2.398773000	4.751222000
H	-1.333060000	2.488915000	3.601854000
H	-2.586076000	3.755687000	3.614132000
C	-3.036371000	-0.192510000	2.935838000
H	-1.998807000	-0.429565000	2.664035000
H	-3.150116000	-0.359333000	4.018532000
H	-3.692127000	-0.910108000	2.423560000
C	2.842883000	0.563943000	3.515991000
H	3.153259000	-0.118103000	4.322632000
H	2.732028000	1.563996000	3.956782000
H	1.852892000	0.245130000	3.162868000
C	5.648715000	1.563958000	2.653426000
H	6.072750000	1.179554000	3.593783000
H	6.440735000	1.530059000	1.890939000
H	5.390283000	2.620519000	2.813662000
C	4.725715000	-1.262244000	1.922948000
H	5.048340000	-1.632452000	2.908613000
H	3.933574000	-1.935056000	1.566936000
H	5.583628000	-1.356796000	1.243202000
C	4.544132000	-0.280841000	-1.330231000
H	5.627859000	-0.104857000	-1.232486000
H	4.308884000	-1.180850000	-0.751723000
H	4.343916000	-0.498341000	-2.387162000
C	3.368504000	1.985744000	-3.224939000
H	4.275837000	2.533196000	-3.527208000
H	3.428864000	0.981333000	-3.662392000
H	2.509975000	2.494898000	-3.681514000
C	2.095978000	4.261602000	-1.425743000
H	2.904498000	4.999527000	-1.553106000
H	1.612086000	4.136769000	-2.402997000
H	1.359056000	4.694276000	-0.739238000
C	2.343809000	3.395545000	1.650193000
H	1.632749000	2.843968000	2.277615000
H	3.205408000	3.681351000	2.272722000
H	1.854120000	4.322042000	1.327090000
C	-1.532461000	4.139425000	0.895236000
H	-2.211673000	4.855602000	1.383549000
H	-0.899013000	3.692097000	1.668355000
H	-0.886161000	4.713481000	0.219927000
C	-1.882063000	4.057595000	-2.274067000
H	-2.606655000	4.876446000	-2.413123000
H	-0.940783000	4.503143000	-1.931957000
H	-1.700223000	3.610164000	-3.259969000

C	-3.697563000	1.550942000	-3.030448000
H	-4.599650000	2.101667000	-3.343414000
H	-2.910699000	1.766120000	-3.765363000
H	-3.928121000	0.479635000	-3.093225000
C	-4.730726000	0.219631000	-0.346331000
H	-4.619555000	-0.376092000	0.565779000
H	-5.752630000	0.632424000	-0.353848000
H	-4.641995000	-0.463080000	-1.200442000
C	-2.976824000	-3.585219000	-0.724649000
H	-3.288969000	-4.642485000	-0.714953000
H	-3.268163000	-3.142584000	0.232754000
H	-3.550273000	-3.080671000	-1.512156000
C	-1.731739000	-3.199222000	-3.572444000
H	-2.187824000	-4.172488000	-3.814305000
H	-2.546889000	-2.466814000	-3.494034000
H	-1.107803000	-2.906185000	-4.424832000
C	1.515917000	-3.361831000	-3.288774000
H	2.035436000	-4.333063000	-3.299164000
H	1.050478000	-3.234099000	-4.273448000
H	2.281543000	-2.581986000	-3.173969000
C	2.219591000	-3.759474000	-0.290216000
H	2.314721000	-3.551017000	0.781122000
H	2.513384000	-4.810703000	-0.447704000
H	2.951244000	-3.137465000	-0.822363000
C	0.459023000	-2.987383000	2.946063000
H	1.540292000	-2.963732000	2.751146000
H	0.086135000	-1.958530000	2.854026000
H	0.323199000	-3.306834000	3.991247000
C	0.289136000	-5.901235000	1.905011000
H	0.251454000	-6.272844000	2.940532000
H	-0.253589000	-6.619561000	1.272987000
H	1.341540000	-5.911631000	1.588330000
C	-2.257967000	-4.301077000	2.460523000
H	-2.769681000	-3.330197000	2.506317000
H	-2.882775000	-4.992547000	1.878937000
H	-2.206929000	-4.690608000	3.489384000

TS3

Ti	0.607217000	1.449623000	-0.563056000
Ti	-1.786591000	-0.046861000	-0.473083000
Ti	0.831630000	-1.357653000	-0.658437000
Si	2.994558000	3.247946000	1.673282000
Si	-3.602438000	-0.065232000	2.797309000
Si	2.944117000	-3.177594000	1.769954000
N	-0.528637000	-0.647472000	0.745232000
N	0.770444000	-0.003355000	0.694449000
C	1.141291000	0.090662000	-2.053303000
H	1.691456000	0.187516000	-2.997247000
C	-0.308857000	-0.014209000	-2.027054000
C	-1.062475000	0.043221000	-3.364898000
H	-0.804493000	0.960145000	-3.915817000
H	-2.155436000	0.022285000	-3.257068000
H	-0.783308000	-0.814871000	-3.995967000
C	1.938227000	3.225156000	0.090736000
C	2.324083000	2.907269000	-1.270450000
C	1.241683000	3.249594000	-2.145260000
C	0.168010000	3.753667000	-1.353687000
C	0.584845000	3.735219000	0.018721000
C	-3.730761000	-0.152040000	0.904207000
C	-3.916028000	0.997618000	0.043329000
C	-4.074843000	0.551313000	-1.307919000
C	-3.959452000	-0.875326000	-1.314740000
C	-3.751638000	-1.307078000	0.041270000
C	2.085260000	-3.162943000	0.077852000
C	0.754048000	-3.679889000	-0.182234000
C	0.492527000	-3.587620000	-1.584150000
C	1.663016000	-3.039571000	-2.217872000

C	2.638353000	-2.791652000	-1.208519000
H	-1.251065000	1.667108000	-0.240455000
C	3.652348000	-4.924432000	2.052455000
H	4.389434000	-5.188889000	1.279980000
H	4.153030000	-4.993622000	3.030332000
H	2.862371000	-5.689499000	2.029083000
C	1.744004000	-2.756746000	3.182100000
H	2.319759000	-2.535081000	4.094271000
H	1.140273000	-1.870495000	2.941314000
H	1.060350000	-3.582820000	3.420628000
C	4.379092000	-1.933977000	1.875149000
H	4.043126000	-0.910425000	1.656452000
H	4.772402000	-1.935772000	2.903611000
H	5.214963000	-2.174893000	1.204678000
C	-0.174699000	-4.282170000	0.848152000
H	0.312944000	-5.120041000	1.368883000
H	-0.481829000	-3.549412000	1.604743000
H	-1.082835000	-4.675608000	0.376411000
C	-0.716578000	-4.106295000	-2.326053000
H	-0.493650000	-5.073179000	-2.806120000
H	-1.569366000	-4.263068000	-1.655310000
H	-1.037188000	-3.415672000	-3.117547000
C	1.839553000	-2.869710000	-3.706323000
H	2.227582000	-3.795189000	-4.162235000
H	0.887206000	-2.637784000	-4.200414000
H	2.542397000	-2.062647000	-3.946927000
C	4.018787000	-2.231046000	-1.468623000
H	4.254055000	-1.380530000	-0.817126000
H	4.791170000	-2.997441000	-1.298406000
H	4.115272000	-1.890497000	-2.506545000
C	-4.196010000	-1.780689000	-2.501531000
H	-3.558045000	-2.672919000	-2.476250000
H	-5.242438000	-2.126038000	-2.522576000
H	-4.006700000	-1.266755000	-3.452946000
C	-4.416848000	1.435913000	-2.483216000
H	-4.219663000	0.940046000	-3.442546000
H	-5.486122000	1.702805000	-2.471772000
H	-3.847716000	2.375380000	-2.470215000
C	-4.127996000	2.426190000	0.487666000
H	-5.196036000	2.609824000	0.689390000
H	-3.573429000	2.658028000	1.402961000
H	-3.815464000	3.139233000	-0.285342000
C	-3.691853000	-2.758012000	0.461835000
H	-2.917513000	-2.942155000	1.212347000
H	-4.655287000	-3.075303000	0.892144000
H	-3.492174000	-3.410099000	-0.397664000
C	-3.221688000	-1.745949000	3.597400000
H	-3.977224000	-2.514073000	3.383589000
H	-2.238900000	-2.126594000	3.285980000
H	-3.190037000	-1.610850000	4.689925000
C	-5.288964000	0.525982000	3.461863000
H	-5.274856000	0.587527000	4.560917000
H	-5.557775000	1.521116000	3.079026000
H	-6.095191000	-0.166088000	3.176831000
C	-2.246698000	1.126638000	3.394796000
H	-2.444935000	2.179753000	3.151828000
H	-2.158406000	1.056517000	4.490649000
H	-1.277863000	0.852588000	2.956336000
C	-0.237023000	4.282488000	1.162577000
H	0.086631000	3.877089000	2.127383000
H	-0.149635000	5.380066000	1.215029000
H	-1.300485000	4.039753000	1.042654000
C	-1.136970000	4.302490000	-1.873676000
H	-1.929691000	4.223159000	-1.120611000
H	-1.037403000	5.367935000	-2.138127000
H	-1.474794000	3.771279000	-2.773342000
C	1.270219000	3.178293000	-3.651026000

H	0.258303000	3.196118000	-4.075086000
H	1.815275000	4.039828000	-4.069003000
H	1.769260000	2.269300000	-4.011477000
C	3.663280000	2.401676000	-1.754489000
H	4.379360000	3.231848000	-1.868629000
H	4.107175000	1.675417000	-1.065748000
H	3.565442000	1.914955000	-2.733005000
C	2.236168000	2.245599000	3.098182000
H	1.304360000	2.680945000	3.485599000
H	2.010889000	1.218108000	2.781067000
H	2.949438000	2.201817000	3.936396000
C	4.751930000	2.575628000	1.395642000
H	5.297539000	3.113749000	0.608519000
H	5.318598000	2.699675000	2.331739000
H	4.766149000	1.504483000	1.150044000
C	3.170032000	5.068973000	2.203719000
H	3.790010000	5.150606000	3.109639000
H	3.649277000	5.667860000	1.415319000
H	2.197627000	5.530750000	2.425293000

Complex 6

Ti	-0.210686000	-1.566943000	-0.625248000
Ti	1.703856000	0.212355000	-0.427556000
Ti	-0.941446000	1.247929000	-0.639193000
Si	-2.326403000	-3.564449000	1.776988000
Si	3.593891000	0.634286000	2.753028000
Si	-3.437258000	2.595803000	1.787130000
N	0.483635000	1.204379000	0.755912000
N	-0.054151000	-0.088203000	0.589223000
C	-1.114694000	-0.271339000	-1.968193000
H	-1.745023000	-0.449262000	-2.847847000
C	0.299118000	0.064513000	-2.095811000
C	0.877616000	0.183194000	-3.510197000
H	0.635242000	-0.713535000	-4.101547000
H	1.967136000	0.297347000	-3.520448000
H	0.451293000	1.048446000	-4.041815000
C	-1.367071000	-3.433459000	0.141727000
C	-1.861247000	-3.177736000	-1.197497000
C	-0.796371000	-3.405605000	-2.128906000
C	0.366826000	-3.786460000	-1.394152000
C	0.026540000	-3.802991000	-0.000560000
C	3.630072000	0.726218000	0.855038000
C	3.973074000	-0.377571000	-0.010410000
C	3.940150000	0.068525000	-1.370987000
C	3.583778000	1.457452000	-1.365572000
C	3.388444000	1.861303000	-0.003572000
C	-2.568900000	2.707321000	0.102543000
C	-1.388760000	3.516687000	-0.150744000
C	-1.116913000	3.487968000	-1.552172000
C	-2.141446000	2.703601000	-2.191314000
C	-3.034762000	2.235187000	-1.188186000
H	1.620906000	-1.598453000	-0.535701000
C	-4.447246000	4.192916000	2.026276000
H	-5.209767000	4.305082000	1.241679000
H	-4.964076000	4.189425000	2.998139000
H	-3.806495000	5.086007000	1.993602000
C	-2.199891000	2.420394000	3.220096000
H	-2.731763000	2.088558000	4.125296000
H	-1.415818000	1.683356000	2.997250000
H	-1.703990000	3.370399000	3.461162000
C	-4.638593000	1.125113000	1.904781000
H	-4.141331000	0.164463000	1.708816000
H	-5.039103000	1.079285000	2.929397000
H	-5.495045000	1.212224000	1.222739000
C	-0.622232000	4.310923000	0.880237000
H	-1.279238000	5.036045000	1.384362000
H	-0.179114000	3.659963000	1.644000000

H	0.190781000	4.879286000	0.412913000
C	-0.045884000	4.258334000	-2.286331000
H	-0.458600000	5.187158000	-2.712827000
H	0.779355000	4.539723000	-1.622325000
H	0.375649000	3.677548000	-3.117257000
C	-2.289584000	2.512728000	-3.680052000
H	-2.939976000	3.292661000	-4.108179000
H	-1.322678000	2.577356000	-4.194294000
H	-2.733765000	1.540498000	-3.927727000
C	-4.271077000	1.410649000	-1.463558000
H	-4.397356000	0.594539000	-0.743363000
H	-5.177678000	2.035480000	-1.416180000
H	-4.230371000	0.965270000	-2.465125000
C	3.584586000	2.384186000	-2.559125000
H	2.737285000	3.080297000	-2.545598000
H	4.507123000	2.986525000	-2.572295000
H	3.545257000	1.831595000	-3.505458000
C	4.362095000	-0.762591000	-2.559332000
H	4.077939000	-0.295319000	-3.510254000
H	5.456729000	-0.889755000	-2.574042000
H	3.914142000	-1.764767000	-2.534289000
C	4.450494000	-1.747130000	0.413628000
H	5.548801000	-1.756847000	0.508038000
H	4.033598000	-2.047789000	1.381145000
H	4.176508000	-2.512786000	-0.322730000
C	3.076890000	3.273295000	0.427265000
H	2.258764000	3.303222000	1.153953000
H	3.958109000	3.747519000	0.887085000
H	2.789178000	3.888801000	-0.433978000
C	3.044544000	2.254973000	3.574828000
H	3.680595000	3.112012000	3.315400000
H	2.006172000	2.502237000	3.315653000
H	3.093479000	2.126603000	4.667560000
C	5.363675000	0.248715000	3.346676000
H	5.400252000	0.192231000	4.445449000
H	5.735149000	-0.708239000	2.953410000
H	6.068129000	1.031927000	3.029699000
C	2.415624000	-0.719408000	3.384555000
H	2.707652000	-1.733624000	3.078231000
H	2.394508000	-0.703265000	4.485783000
H	1.393449000	-0.541266000	3.023912000
C	0.966870000	-4.237931000	1.099971000
H	0.667798000	-3.834959000	2.074493000
H	0.990570000	-5.336556000	1.186457000
H	1.992308000	-3.898967000	0.904382000
C	1.691931000	-4.199462000	-1.985304000
H	2.515064000	-4.020181000	-1.283644000
H	1.690511000	-5.274295000	-2.229553000
H	1.914846000	-3.651235000	-2.909657000
C	-0.906747000	-3.338998000	-3.631406000
H	0.075189000	-3.201451000	-4.101461000
H	-1.335361000	-4.271677000	-4.032193000
H	-1.552742000	-2.514025000	-3.958891000
C	-3.275600000	-2.843089000	-1.607931000
H	-3.886947000	-3.756325000	-1.692296000
H	-3.769118000	-2.178520000	-0.891782000
H	-3.291743000	-2.347284000	-2.586634000
C	-1.694274000	-2.362212000	3.106609000
H	-0.642111000	-2.534178000	3.372473000
H	-1.775082000	-1.318683000	2.772754000
H	-2.290321000	-2.473819000	4.026045000
C	-4.191854000	-3.254245000	1.570287000
H	-4.649725000	-3.915749000	0.821945000
H	-4.682892000	-3.459725000	2.534381000
H	-4.434301000	-2.217521000	1.299724000
C	-2.148313000	-5.350873000	2.413659000
H	-2.730484000	-5.487086000	3.337994000

H	-2.523945000	-6.072962000	1.673753000
H	-1.106266000	-5.617237000	2.637105000

TS4

Ti	-0.073886000	1.413932000	0.584661000
Ti	1.337541000	-0.719838000	-0.502703000
Ti	-1.329661000	-0.956410000	0.645221000
Si	-0.812121000	4.155892000	-1.787331000
Si	4.982382000	-1.243483000	0.558087000
Si	-4.226788000	-1.868720000	-1.571151000
N	-0.478281000	-0.183313000	-0.831616000
N	0.993317000	1.120068000	-0.919511000
C	0.537974000	-1.695024000	1.199916000
H	0.865200000	-2.577826000	1.763049000
C	0.662876000	-0.380352000	1.717446000
C	1.231134000	-0.181789000	3.126306000
H	1.359671000	-1.146470000	3.644304000
H	0.566494000	0.441885000	3.739853000
H	2.209751000	0.315692000	3.104760000
C	-0.357623000	3.692879000	-0.000734000
C	-1.316796000	3.403212000	1.039498000
C	-0.610124000	3.125151000	2.257962000
C	0.787594000	3.238347000	1.986500000
C	0.948023000	3.583141000	0.601396000
C	3.591263000	-1.500938000	-0.702961000
C	2.721767000	-2.648650000	-0.881365000
C	1.940436000	-2.444655000	-2.064034000
C	2.322663000	-1.188412000	-2.641889000
C	3.337096000	-0.616886000	-1.823359000
C	-3.392196000	-1.945745000	0.136597000
C	-2.512868000	-3.013125000	0.566828000
C	-2.182193000	-2.822873000	1.942761000
C	-2.837735000	-1.628064000	2.388895000
C	-3.594987000	-1.096629000	1.289311000
H	-1.635918000	0.714331000	1.270038000
C	2.705470000	-3.918519000	-0.064156000
H	3.528988000	-4.587194000	-0.363460000
H	2.809159000	-3.725822000	1.008601000
H	1.768574000	-4.470404000	-0.213033000
C	0.959799000	-3.415664000	-2.675295000
H	1.454485000	-4.034085000	-3.441922000
H	0.537288000	-4.097644000	-1.928092000
H	0.126191000	-2.894267000	-3.162229000
C	4.025282000	0.686276000	-2.146740000
H	4.635305000	1.047403000	-1.312269000
H	4.686866000	0.568997000	-3.019924000
H	3.289364000	1.466632000	-2.384857000
C	1.772420000	-0.579466000	-3.907151000
H	1.700330000	0.511698000	-3.819156000
H	2.422372000	-0.808480000	-4.767425000
H	0.770400000	-0.962556000	-4.137208000
C	-2.975262000	-1.878266000	-3.003140000
H	-2.471306000	-2.846738000	-3.130168000
H	-3.496760000	-1.657148000	-3.947602000
H	-2.201557000	-1.113054000	-2.850834000
C	-5.302531000	-0.319466000	-1.806841000
H	-5.779071000	-0.381322000	-2.797733000
H	-6.104877000	-0.230267000	-1.062236000
H	-4.711029000	0.606730000	-1.789382000
C	-5.365033000	-3.388648000	-1.719684000
H	-5.881526000	-3.394169000	-2.691667000
H	-4.806810000	-4.332012000	-1.636012000
H	-6.133671000	-3.388426000	-0.932900000
C	-2.072940000	-4.204987000	-0.249943000
H	-2.102587000	-3.998971000	-1.325148000
H	-1.049723000	-4.510750000	0.005533000
H	-2.730910000	-5.068067000	-0.058548000

C	-1.405400000	-3.776758000	2.814175000
H	-2.089379000	-4.466942000	3.334359000
H	-0.707928000	-4.386511000	2.226711000
H	-0.825098000	-3.248781000	3.582308000
C	-2.808719000	-1.099240000	3.801635000
H	-3.593624000	-1.572744000	4.414057000
H	-1.845631000	-1.304225000	4.286695000
H	-2.972010000	-0.015766000	3.834092000
C	-4.531961000	0.083073000	1.401792000
H	-4.489521000	0.736202000	0.525223000
H	-5.573263000	-0.258968000	1.515998000
H	-4.288862000	0.690209000	2.282106000
C	-1.931591000	2.851479000	-2.603090000
H	-2.067828000	3.099352000	-3.667749000
H	-1.472443000	1.855370000	-2.539420000
H	-2.933121000	2.791947000	-2.153523000
C	-1.733708000	5.824146000	-1.734198000
H	-1.100665000	6.614896000	-1.305015000
H	-2.021225000	6.141276000	-2.748419000
H	-2.651548000	5.772269000	-1.131257000
C	0.697160000	4.361638000	-2.919690000
H	0.346256000	4.662332000	-3.919429000
H	1.401001000	5.129922000	-2.572279000
H	1.242587000	3.414307000	-3.027499000
C	-2.818161000	3.540821000	0.943941000
H	-3.123928000	4.569110000	1.197816000
H	-3.187954000	3.328408000	-0.065449000
H	-3.330693000	2.863296000	1.636639000
C	2.278620000	3.865104000	-0.052612000
H	2.365614000	3.354438000	-1.017317000
H	2.411511000	4.945247000	-0.221715000
H	3.107111000	3.526830000	0.582135000
C	1.896494000	3.196983000	3.010674000
H	2.804099000	2.715942000	2.624993000
H	2.172673000	4.221685000	3.307531000
H	1.594212000	2.664254000	3.919897000
C	-1.248981000	2.890254000	3.603599000
H	-0.586467000	2.339532000	4.283255000
H	-1.493731000	3.848052000	4.091481000
H	-2.181664000	2.319889000	3.511385000
C	4.925572000	-2.473203000	2.008380000
H	5.057848000	-3.516883000	1.692940000
H	5.748580000	-2.233146000	2.699722000
H	3.988870000	-2.404551000	2.580210000
C	4.934595000	0.500799000	1.330973000
H	5.393697000	1.266493000	0.690150000
H	3.901248000	0.815804000	1.534018000
H	5.483234000	0.503069000	2.285608000
C	6.646663000	-1.470829000	-0.337486000
H	7.491802000	-1.304610000	0.347913000
H	6.742524000	-2.486984000	-0.747232000
H	6.752695000	-0.766396000	-1.175096000
E			
Ti	-0.027141000	1.393555000	0.731329000
Ti	1.468803000	-0.591235000	-0.320055000
Ti	-1.258016000	-1.004727000	0.656739000
Si	-1.081075000	3.962169000	-1.871412000
Si	5.159794000	-1.014062000	0.348671000
Si	-4.123708000	-1.922490000	-1.632983000
N	-0.343798000	0.010557000	-0.640993000
N	1.761134000	0.900467000	0.676663000
C	0.597780000	-1.824029000	1.222821000
H	1.081468000	-2.740354000	1.579844000
C	0.510256000	-0.647914000	1.947137000
C	1.027806000	-0.392760000	3.348355000
H	1.564562000	0.561016000	3.409521000

H	1.700305000	-1.193099000	3.693341000
H	0.174014000	-0.332278000	4.040516000
C	-0.580146000	3.556155000	-0.084124000
C	-1.520290000	3.297019000	0.979843000
C	-0.803573000	3.188821000	2.216019000
C	0.581212000	3.441166000	1.944238000
C	0.727030000	3.655178000	0.543775000
C	3.705369000	-1.249339000	-0.842177000
C	2.917945000	-2.462128000	-0.946309000
C	2.000371000	-2.325334000	-2.032711000
C	2.175477000	-1.024755000	-2.597995000
C	3.229750000	-0.364880000	-1.879848000
C	-3.291190000	-2.013346000	0.073572000
C	-2.405316000	-3.084942000	0.491615000
C	-2.140878000	-2.952080000	1.888132000
C	-2.829773000	-1.791084000	2.357967000
C	-3.550840000	-1.222324000	1.256199000
H	-1.692199000	0.626800000	1.264925000
C	3.126544000	-3.738431000	-0.164254000
H	3.824233000	-4.409558000	-0.690571000
H	3.544990000	-3.546280000	0.830870000
H	2.186048000	-4.290132000	-0.029624000
C	1.070796000	-3.390336000	-2.554682000
H	1.537108000	-3.939703000	-3.389141000
H	0.821240000	-4.125557000	-1.780356000
H	0.132421000	-2.963363000	-2.930765000
C	3.773362000	0.999426000	-2.238417000
H	3.966840000	1.610188000	-1.351495000
H	4.715088000	0.909674000	-2.803371000
H	3.066990000	1.547787000	-2.874603000
C	1.436138000	-0.487776000	-3.800293000
H	1.336095000	0.604227000	-3.765237000
H	1.966132000	-0.740959000	-4.732994000
H	0.424804000	-0.907502000	-3.868695000
C	-2.868419000	-1.838006000	-3.059682000
H	-2.321671000	-2.780145000	-3.206354000
H	-3.394280000	-1.618434000	-4.001917000
H	-2.130268000	-1.042251000	-2.889046000
C	-5.273047000	-0.421628000	-1.828001000
H	-5.739672000	-0.475337000	-2.824065000
H	-6.083619000	-0.399615000	-1.087244000
H	-4.731445000	0.532789000	-1.775038000
C	-5.191869000	-3.486302000	-1.835244000
H	-5.709545000	-3.479249000	-2.806628000
H	-4.593101000	-4.406784000	-1.786238000
H	-5.958585000	-3.548013000	-1.049027000
C	-1.929800000	-4.242544000	-0.353890000
H	-1.914210000	-3.992080000	-1.419827000
H	-0.917488000	-4.559276000	-0.071124000
H	-2.594055000	-5.112610000	-0.226638000
C	-1.352091000	-3.914645000	2.738779000
H	-2.025568000	-4.632970000	3.233269000
H	-0.638534000	-4.492705000	2.139156000
H	-0.786446000	-3.398472000	3.525773000
C	-2.873891000	-1.308096000	3.787661000
H	-3.784215000	-1.664691000	4.296265000
H	-2.014507000	-1.676857000	4.361865000
H	-2.870550000	-0.212205000	3.847976000
C	-4.535906000	-0.087789000	1.401269000
H	-4.525666000	0.588694000	0.542545000
H	-5.560125000	-0.480924000	1.507938000
H	-4.317614000	0.504067000	2.298330000
C	-2.139000000	2.593889000	-2.662069000
H	-2.241291000	2.780692000	-3.742601000
H	-1.668718000	1.610470000	-2.524629000
H	-3.154521000	2.541824000	-2.244890000
C	-2.075083000	5.587396000	-1.844493000

H	-1.478002000	6.411431000	-1.426977000
H	-2.375872000	5.875405000	-2.863507000
H	-2.989873000	5.502731000	-1.240958000
C	0.401700000	4.233851000	-3.031000000
H	0.014014000	4.496489000	-4.027890000
H	1.057987000	5.053175000	-2.707959000
H	1.016049000	3.330037000	-3.149077000
C	-3.023717000	3.279156000	0.863656000
H	-3.428035000	4.299469000	0.966940000
H	-3.357699000	2.887848000	-0.103871000
H	-3.480559000	2.664978000	1.647754000
C	2.049734000	3.976643000	-0.105783000
H	2.104010000	3.611858000	-1.135047000
H	2.224649000	5.065186000	-0.123056000
H	2.871202000	3.511315000	0.453087000
C	1.708551000	3.471602000	2.945661000
H	2.549923000	2.849365000	2.609455000
H	2.083661000	4.497723000	3.084007000
H	1.386190000	3.107177000	3.929639000
C	-1.420559000	2.971646000	3.576853000
H	-0.717157000	2.494386000	4.271725000
H	-1.727999000	3.928858000	4.028346000
H	-2.312333000	2.334663000	3.516423000
C	4.646394000	-1.199481000	2.171347000
H	4.214751000	-2.181656000	2.411009000
H	5.520900000	-1.056824000	2.825534000
H	3.901363000	-0.433753000	2.426865000
C	5.988781000	0.689779000	0.204029000
H	6.359669000	0.904957000	-0.807224000
H	5.311029000	1.501984000	0.501419000
H	6.854007000	0.715546000	0.885042000
C	6.480838000	-2.325493000	-0.062930000
H	7.355454000	-2.217179000	0.596882000
H	6.102279000	-3.350641000	0.055906000
H	6.831526000	-2.221947000	-1.100467000

TS5

Ti	-0.041055000	1.403185000	0.715556000
Ti	1.463484000	-0.609529000	-0.309647000
Ti	-1.272207000	-0.976328000	0.667867000
Si	-1.123268000	3.930193000	-1.911315000
Si	5.175039000	-0.994706000	0.341261000
Si	-4.105974000	-2.000860000	-1.619812000
N	-0.340273000	0.016805000	-0.646730000
N	1.743847000	0.856792000	0.742983000
C	0.571801000	-1.778408000	1.226520000
H	1.024160000	-2.689027000	1.634642000
C	0.531556000	-0.558112000	1.916691000
C	1.043748000	-0.329667000	3.326861000
H	1.408161000	0.692604000	3.475002000
H	1.850027000	-1.029622000	3.592011000
H	0.208394000	-0.488035000	4.026551000
C	-0.582256000	3.557476000	-0.128975000
C	-1.496761000	3.330615000	0.963453000
C	-0.749587000	3.240007000	2.184487000
C	0.629268000	3.469829000	1.872929000
C	0.742219000	3.646688000	0.463672000
C	3.704418000	-1.261352000	-0.822935000
C	2.924589000	-2.481032000	-0.891946000
C	2.004263000	-2.379979000	-1.980338000
C	2.168922000	-1.094357000	-2.581171000
C	3.217825000	-0.407320000	-1.881407000
C	-3.293670000	-2.017775000	0.098764000
C	-2.408115000	-3.066189000	0.572470000
C	-2.161271000	-2.872777000	1.965193000
C	-2.861783000	-1.696430000	2.376688000
C	-3.571262000	-1.178075000	1.242560000

H	-1.710244000	0.673692000	1.236793000
C	3.138826000	-3.732445000	-0.072167000
H	3.836641000	-4.418195000	-0.579167000
H	3.558753000	-3.508523000	0.915671000
H	2.199764000	-4.281372000	0.082023000
C	1.082857000	-3.466389000	-2.472200000
H	1.554459000	-4.035418000	-3.290337000
H	0.837842000	-4.181625000	-1.677956000
H	0.141913000	-3.057418000	-2.861414000
C	3.750737000	0.950208000	-2.280043000
H	3.967784000	1.578506000	-1.411152000
H	4.678087000	0.850077000	-2.866814000
H	3.028284000	1.486222000	-2.908811000
C	1.424895000	-0.593294000	-3.796010000
H	1.303869000	0.497181000	-3.780985000
H	1.963550000	-0.852776000	-4.721995000
H	0.422014000	-1.033219000	-3.861276000
C	-2.833506000	-1.957740000	-3.033167000
H	-2.279079000	-2.900933000	-3.138461000
H	-3.348479000	-1.775981000	-3.989354000
H	-2.102479000	-1.151376000	-2.882343000
C	-5.268226000	-0.521002000	-1.884954000
H	-5.730762000	-0.623613000	-2.879102000
H	-6.081530000	-0.473691000	-1.148448000
H	-4.735816000	0.439893000	-1.873028000
C	-5.154914000	-3.582876000	-1.774650000
H	-5.659906000	-3.618983000	-2.752041000
H	-4.547392000	-4.494219000	-1.682247000
H	-5.931156000	-3.622303000	-0.996396000
C	-1.912406000	-4.253890000	-0.217936000
H	-1.896712000	-4.052244000	-1.294305000
H	-0.896150000	-4.540737000	0.082258000
H	-2.563561000	-5.127530000	-0.053104000
C	-1.379820000	-3.795197000	2.865664000
H	-2.057564000	-4.489563000	3.387791000
H	-0.662428000	-4.400712000	2.298667000
H	-0.819391000	-3.243671000	3.632144000
C	-2.929606000	-1.155588000	3.784668000
H	-3.849271000	-1.490773000	4.291013000
H	-2.081231000	-1.501824000	4.388467000
H	-2.925071000	-0.058271000	3.800955000
C	-4.558351000	-0.038745000	1.325017000
H	-4.523764000	0.611336000	0.446362000
H	-5.585916000	-0.426850000	1.416016000
H	-4.363071000	0.580493000	2.208554000
C	-2.214042000	2.556734000	-2.646493000
H	-2.348467000	2.726236000	-3.726360000
H	-1.746311000	1.572370000	-2.506757000
H	-3.216466000	2.519401000	-2.197148000
C	-2.100352000	5.565761000	-1.894970000
H	-1.484681000	6.392446000	-1.511021000
H	-2.424981000	5.834905000	-2.911815000
H	-2.999708000	5.503405000	-1.266025000
C	0.334190000	4.161918000	-3.111032000
H	-0.073907000	4.410847000	-4.103252000
H	1.007541000	4.979053000	-2.818931000
H	0.934818000	3.248600000	-3.226809000
C	-3.003231000	3.333814000	0.889033000
H	-3.389518000	4.359905000	1.003553000
H	-3.369522000	2.947414000	-0.068556000
H	-3.447065000	2.725753000	1.685496000
C	2.053822000	3.932547000	-0.224859000
H	2.078666000	3.542812000	-1.246173000
H	2.243989000	5.017549000	-0.273787000
H	2.881932000	3.470318000	0.326955000
C	1.783309000	3.510964000	2.842710000
H	2.588456000	2.834174000	2.523310000

H	2.202829000	4.526803000	2.909979000
H	1.472649000	3.219072000	3.854209000
C	-1.336817000	3.061281000	3.564088000
H	-0.620713000	2.597901000	4.255143000
H	-1.630027000	4.031366000	3.997230000
H	-2.232944000	2.427923000	3.540243000
C	4.692394000	-1.119421000	2.176852000
H	4.241718000	-2.084308000	2.449463000
H	5.582164000	-0.981396000	2.811101000
H	3.970482000	-0.329344000	2.424359000
C	6.011572000	0.699102000	0.129998000
H	6.364692000	0.881947000	-0.893940000
H	5.346573000	1.525668000	0.416653000
H	6.889941000	0.738205000	0.793325000
C	6.484739000	-2.323454000	-0.050767000
H	7.371214000	-2.196160000	0.589550000
H	6.105919000	-3.342950000	0.108527000
H	6.817108000	-2.255165000	-1.097219000

F

Ti	-0.003059000	1.446591000	0.584288000
Ti	1.301429000	-0.902308000	-0.243276000
Ti	-1.452450000	-0.752086000	0.700506000
Si	-0.678587000	4.036989000	-2.064598000
Si	5.086139000	-1.146025000	0.313650000
Si	-4.030346000	-2.041404000	-1.695792000
N	-0.344377000	0.009230000	-0.679467000
N	1.587294000	0.479173000	1.037093000
C	0.238713000	-1.727597000	1.254745000
H	0.390968000	-2.593795000	1.907019000
C	0.590128000	-0.350697000	1.842620000
C	0.902435000	-0.328773000	3.339588000
H	1.093763000	0.696165000	3.679874000
H	1.795098000	-0.933288000	3.564975000
H	0.060124000	-0.736210000	3.914486000
C	-0.238244000	3.634832000	-0.262529000
C	-1.097683000	3.558835000	0.893302000
C	-0.283355000	3.381383000	2.065441000
C	1.088042000	3.397434000	1.658516000
C	1.121941000	3.524787000	0.241669000
C	3.548179000	-1.611793000	-0.693177000
C	2.779132000	-2.819935000	-0.486088000
C	1.816515000	-2.943159000	-1.535189000
C	1.949794000	-1.810640000	-2.396398000
C	3.009795000	-0.989843000	-1.882690000
C	-3.438633000	-1.822834000	0.098913000
C	-2.736987000	-2.750263000	0.967209000
C	-2.679637000	-2.192941000	2.281902000
C	-3.318942000	-0.914238000	2.253756000
C	-3.798250000	-0.688410000	0.921173000
H	-1.700340000	1.010216000	1.111219000
C	6.377348000	-2.526096000	0.065790000
H	6.643262000	-2.635790000	-0.995997000
H	7.301226000	-2.298891000	0.619722000
H	6.013219000	-3.502084000	0.416937000
C	5.894378000	0.480610000	-0.251291000
H	5.249949000	1.353144000	-0.074141000
H	6.814269000	0.631105000	0.335274000
H	6.179316000	0.475225000	-1.312162000
C	4.730187000	-0.950348000	2.170823000
H	5.634301000	-0.594620000	2.689474000
H	3.930983000	-0.212138000	2.322162000
H	4.421358000	-1.885793000	2.658672000
C	3.511247000	0.260735000	-2.569736000
H	3.809720000	1.035657000	-1.856842000
H	4.386770000	0.034929000	-3.199913000
H	2.741565000	0.685458000	-3.226292000

C	1.162516000	-1.566500000	-3.662083000
H	1.031212000	-0.496012000	-3.862442000
H	1.672254000	-2.007123000	-4.534274000
H	0.161541000	-2.013290000	-3.605557000
C	0.888694000	-4.112772000	-1.740907000
H	-0.013941000	-3.823930000	-2.294368000
H	1.385838000	-4.906581000	-2.322353000
H	0.574093000	-4.553016000	-0.786735000
C	3.010202000	-3.870334000	0.574896000
H	3.658553000	-4.676224000	0.194247000
H	3.491273000	-3.452551000	1.466497000
H	2.066520000	-4.333834000	0.892932000
C	2.403995000	3.613378000	-0.551296000
H	2.250777000	3.390365000	-1.613017000
H	2.833002000	4.626688000	-0.484776000
H	3.155819000	2.913328000	-0.162891000
C	2.306464000	3.284307000	2.537923000
H	2.892041000	2.391104000	2.276389000
H	2.954906000	4.166088000	2.421772000
H	2.034912000	3.212567000	3.598559000
C	-0.794544000	3.323127000	3.485604000
H	-0.056015000	2.875635000	4.162274000
H	-1.020101000	4.332724000	3.865672000
H	-1.713818000	2.728654000	3.562250000
C	-2.592856000	3.765626000	0.940215000
H	-2.834855000	4.840922000	0.922642000
H	-3.106863000	3.294963000	0.097215000
H	-3.014479000	3.352065000	1.864805000
C	0.062682000	5.742206000	-2.476726000
H	-0.163173000	6.026271000	-3.515920000
H	-0.347860000	6.522865000	-1.819579000
H	1.155686000	5.753701000	-2.359563000
C	-2.552197000	4.130872000	-2.376239000
H	-3.057156000	4.885227000	-1.757927000
H	-2.713600000	4.407195000	-3.429975000
H	-3.049996000	3.164139000	-2.214201000
C	0.000165000	2.748539000	-3.289160000
H	1.097322000	2.751073000	-3.354081000
H	-0.316648000	1.735956000	-3.002907000
H	-0.386999000	2.957730000	-4.298810000
C	-3.405946000	-0.655165000	-2.838367000
H	-3.663908000	-0.888651000	-3.883365000
H	-3.848954000	0.323314000	-2.604553000
H	-2.314921000	-0.544502000	-2.768843000
C	-3.487542000	-3.690477000	-2.471632000
H	-3.817141000	-4.564224000	-1.892947000
H	-3.945880000	-3.766339000	-3.470106000
H	-2.399809000	-3.763275000	-2.609217000
C	-5.934677000	-2.044749000	-1.686593000
H	-6.322467000	-2.200148000	-2.705034000
H	-6.326027000	-2.854688000	-1.053583000
H	-6.354143000	-1.100314000	-1.313674000
C	-4.655104000	0.485496000	0.511135000
H	-4.554743000	0.714104000	-0.556140000
H	-5.718785000	0.274176000	0.707582000
H	-4.388672000	1.389786000	1.069900000
C	-3.542995000	-0.009514000	3.440606000
H	-3.640341000	1.038039000	3.130953000
H	-4.466544000	-0.285352000	3.975129000
H	-2.716450000	-0.068240000	4.160606000
C	-2.135185000	-2.881059000	3.508131000
H	-1.882378000	-2.162891000	4.298136000
H	-2.882978000	-3.575071000	3.924416000
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C	-2.231600000	-4.130443000	0.624833000
H	-3.024374000	-4.882837000	0.769256000
H	-1.892711000	-4.201913000	-0.412094000

H	-1.391258000	-4.412337000	1.272322000
TS6			
Ti	0.151466000	1.350492000	0.757283000
Ti	1.227320000	-1.118852000	-0.043295000
Ti	-1.588998000	-0.820274000	0.528566000
Si	-0.068319000	3.965007000	-1.900039000
Si	5.042487000	-0.851215000	-0.553291000
Si	-4.463973000	-0.731194000	-1.835489000
N	-0.262766000	-0.026837000	-0.584369000
N	1.755939000	0.297429000	1.102683000
C	-0.037017000	-1.494931000	1.627016000
H	-0.054138000	-2.307314000	2.365975000
C	0.896050000	-0.357880000	2.060832000
C	1.412572000	-0.457167000	3.493121000
H	2.056629000	0.396481000	3.729463000
H	2.000595000	-1.379551000	3.635712000
H	0.575844000	-0.482317000	4.205078000
C	0.119840000	3.513216000	-0.066581000
C	-0.885904000	3.456683000	0.972597000
C	-0.231728000	3.247457000	2.235937000
C	1.178438000	3.222524000	2.004644000
C	1.400321000	3.360976000	0.606190000
C	3.402223000	-1.779302000	-0.758721000
C	2.926623000	-2.809715000	0.134440000
C	1.797013000	-3.463176000	-0.456740000
C	1.557675000	-2.854297000	-1.731002000
C	2.522291000	-1.815399000	-1.911453000
C	-3.771863000	-1.259834000	-0.148597000
C	-3.129006000	-2.538070000	0.102090000
C	-2.866887000	-2.663571000	1.504421000
C	-3.320650000	-1.469691000	2.141921000
C	-3.883388000	-0.612496000	1.141879000
H	-1.597807000	0.864007000	1.259597000
C	6.443045000	-2.106412000	-0.864754000
H	6.384306000	-2.530072000	-1.878229000
H	7.430164000	-1.630852000	-0.757487000
H	6.400646000	-2.944895000	-0.154157000
C	5.266288000	-0.098311000	1.179953000
H	6.026086000	0.697931000	1.142673000
H	4.321977000	0.338374000	1.533324000
H	5.605456000	-0.832975000	1.924321000
C	5.264011000	0.561461000	-1.808596000
H	4.487053000	1.333061000	-1.718739000
H	6.232182000	1.049026000	-1.613987000
H	5.278292000	0.210980000	-2.849491000
C	3.534436000	-3.212242000	1.458213000
H	4.282633000	-4.010200000	1.321979000
H	4.032065000	-2.370212000	1.951054000
H	2.771749000	-3.599830000	2.147864000
C	1.101592000	-4.676491000	0.107810000
H	1.675092000	-5.592376000	-0.110307000
H	0.989686000	-4.610459000	1.197654000
H	0.101454000	-4.807135000	-0.322919000
C	0.514218000	-3.264436000	-2.742859000
H	0.977171000	-3.803618000	-3.584758000
H	-0.233502000	-3.932444000	-2.299662000
H	-0.018094000	-2.399064000	-3.160157000
C	2.620319000	-0.972520000	-3.163945000
H	2.839709000	0.077944000	-2.945104000
H	3.418741000	-1.345975000	-3.825312000
H	1.682754000	-1.004788000	-3.732717000
C	-2.933459000	-3.650401000	-0.903079000
H	-3.828241000	-4.292660000	-0.941009000
H	-2.759319000	-3.269550000	-1.915792000
H	-2.085951000	-4.293195000	-0.635118000
C	-2.318942000	-3.882994000	2.198607000

H	-3.133201000	-4.577857000	2.459844000
H	-1.609152000	-4.429008000	1.565590000
H	-1.802056000	-3.621277000	3.130988000
C	-3.247311000	-1.175534000	3.619848000
H	-4.191770000	-1.438059000	4.123252000
H	-2.445004000	-1.748205000	4.101611000
H	-3.055272000	-0.112031000	3.811459000
C	-4.579848000	0.691316000	1.453189000
H	-4.419175000	1.446163000	0.679080000
H	-5.666525000	0.532389000	1.545808000
H	-4.226862000	1.107359000	2.404745000
C	-5.276603000	0.987266000	-1.807350000
H	-5.697507000	1.185088000	-2.805554000
H	-6.100334000	1.060323000	-1.084270000
H	-4.561479000	1.793699000	-1.592649000
C	-5.810675000	-1.975655000	-2.350449000
H	-6.250676000	-1.689987000	-3.318161000
H	-5.418357000	-2.996874000	-2.454827000
H	-6.624258000	-2.007428000	-1.610875000
C	-3.111779000	-0.679758000	-3.174114000
H	-2.258334000	-0.066559000	-2.851322000
H	-2.723645000	-1.675720000	-3.431057000
H	-3.518389000	-0.241076000	-4.098838000
C	-1.881485000	4.140400000	-2.446538000
H	-2.436021000	4.894497000	-1.871983000
H	-1.895305000	4.455123000	-3.501809000
H	-2.429855000	3.189769000	-2.384730000
C	0.775837000	5.650952000	-2.170533000
H	1.844100000	5.622878000	-1.912892000
H	0.695485000	5.964687000	-3.222575000
H	0.307891000	6.431092000	-1.552166000
C	0.713595000	2.676380000	-3.059981000
H	0.313691000	1.674577000	-2.850345000
H	0.480254000	2.928269000	-4.106541000
H	1.808100000	2.623057000	-2.974974000
C	-2.368435000	3.703869000	0.824101000
H	-2.576557000	4.783887000	0.750850000
H	-2.784169000	3.226419000	-0.069176000
H	-2.916866000	3.322122000	1.693035000
C	-0.916710000	3.163296000	3.578861000
H	-1.139656000	4.167597000	3.974400000
H	-1.866082000	2.616080000	3.513259000
H	-0.289454000	2.648729000	4.317635000
C	2.271487000	3.094739000	3.032459000
H	2.803972000	4.051939000	3.150486000
H	1.877158000	2.814466000	4.016927000
H	3.009963000	2.339253000	2.730829000
C	2.773524000	3.404979000	-0.018211000
H	2.733160000	3.268361000	-1.104751000
H	3.259864000	4.375195000	0.174450000
H	3.420571000	2.620758000	0.396847000

Complex 5

Ti	-0.538366000	1.310281000	-0.401810000
H	-1.965095000	0.185850000	-0.330362000
Ti	1.601970000	-0.261806000	0.371174000
Ti	-0.962841000	-1.207552000	0.467058000
Si	-1.688953000	4.572496000	0.972061000
Si	4.952303000	-1.305396000	-1.201239000
Si	-3.992847000	-2.974719000	-1.138312000
N	0.831271000	-2.033780000	0.289967000
N	-0.036879000	0.395504000	1.155934000
C	0.265120000	-0.374410000	-1.414720000
H	0.156149000	-0.225212000	-2.494814000
C	0.607664000	-1.744065000	-1.074099000
C	0.912893000	-2.802829000	-2.125969000
H	0.276226000	-2.671242000	-3.010668000

H	0.750396000	-3.804847000	-1.711980000
H	1.960574000	-2.740827000	-2.453059000
C	-1.242592000	3.527195000	-0.546812000
C	-2.198754000	2.725698000	-1.286143000
C	-1.551874000	2.192125000	-2.447596000
C	-0.198208000	2.654139000	-2.452315000
C	0.001320000	3.468179000	-1.295135000
C	-3.677281000	2.597933000	-1.002560000
H	-4.070879000	1.637045000	-1.356163000
H	-4.238866000	3.394699000	-1.517148000
H	-3.901781000	2.673866000	0.067419000
C	-2.208065000	1.361179000	-3.522216000
H	-1.489231000	0.695192000	-4.018521000
H	-2.648955000	2.002148000	-4.303111000
H	-3.013146000	0.736509000	-3.115375000
C	0.806750000	2.397310000	-3.547411000
H	1.836814000	2.423934000	-3.172392000
H	0.720044000	3.156110000	-4.342049000
H	0.652663000	1.417782000	-4.019741000
C	1.246709000	4.283129000	-1.039893000
H	1.525369000	4.307448000	0.018126000
H	1.093023000	5.326282000	-1.361773000
H	2.097980000	3.889190000	-1.605578000
C	-0.227110000	5.583904000	1.647586000
H	0.583333000	4.952436000	2.037418000
H	-0.592022000	6.198568000	2.485357000
H	0.200935000	6.267541000	0.901919000
C	-3.045122000	5.815748000	0.481013000
H	-2.702102000	6.474778000	-0.330103000
H	-3.312667000	6.452908000	1.337894000
H	-3.963617000	5.319859000	0.138012000
C	-2.318429000	3.499104000	2.413677000
H	-3.256827000	2.976484000	2.179947000
H	-2.506208000	4.128645000	3.297622000
H	-1.575451000	2.737401000	2.691271000
C	3.961575000	-0.514901000	0.203699000
C	3.530755000	-1.127878000	1.445210000
C	3.015541000	-0.101856000	2.295747000
C	3.147231000	1.157826000	1.619493000
C	3.728527000	0.912961000	0.341898000
C	3.654657000	-2.583684000	1.827630000
H	3.129390000	-2.784277000	2.769269000
H	4.709515000	-2.863236000	1.975293000
H	3.225159000	-3.244114000	1.066085000
C	2.472802000	-0.258736000	3.695969000
H	1.615082000	0.405334000	3.864986000
H	3.242562000	-0.007903000	4.443998000
H	2.144501000	-1.286087000	3.893998000
C	2.773928000	2.483004000	2.235031000
H	2.904464000	3.310688000	1.528563000
H	3.405242000	2.695605000	3.112317000
H	1.727659000	2.486676000	2.572058000
C	4.169363000	1.973038000	-0.641628000
H	3.772707000	1.802111000	-1.649874000
H	5.267954000	1.995141000	-0.719429000
H	3.846000000	2.969202000	-0.320653000
C	4.859976000	-3.205252000	-1.210994000
H	5.338093000	-3.648476000	-0.326966000
H	5.396875000	-3.579512000	-2.096755000
H	3.831435000	-3.587009000	-1.261350000
C	4.378096000	-0.691626000	-2.913480000
H	3.282554000	-0.692310000	-3.008656000
H	4.782031000	-1.347214000	-3.700425000
H	4.729591000	0.327126000	-3.128365000
C	6.788200000	-0.840706000	-0.987608000
H	6.945603000	0.247209000	-1.011191000
H	7.399897000	-1.281330000	-1.789967000

H	7.180203000	-1.209511000	-0.028439000
C	-2.956169000	-2.557007000	0.394566000
C	-1.890165000	-3.391374000	0.893388000
C	-1.420152000	-2.854435000	2.130730000
C	-2.197590000	-1.684872000	2.432390000
C	-3.146150000	-1.506096000	1.376398000
C	-1.332669000	-4.652052000	0.281028000
H	-1.609157000	-4.756976000	-0.774358000
H	-1.706605000	-5.541482000	0.813473000
H	-0.235858000	-4.660717000	0.349047000
C	-0.330510000	-3.463431000	2.974165000
H	0.551972000	-3.693273000	2.362130000
H	-0.676297000	-4.399625000	3.440810000
H	-0.020755000	-2.787458000	3.780488000
C	-2.086708000	-0.847294000	3.683279000
H	-1.065921000	-0.860611000	4.084069000
H	-2.761211000	-1.225572000	4.468543000
H	-2.347849000	0.200210000	3.492501000
C	-4.224232000	-0.449398000	1.393176000
H	-3.911288000	0.420229000	1.983967000
H	-5.145340000	-0.844097000	1.852802000
H	-4.473602000	-0.096638000	0.389390000
C	-5.426939000	-1.764091000	-1.444939000
H	-6.108127000	-1.681464000	-0.587148000
H	-6.016047000	-2.135773000	-2.297987000
H	-5.082312000	-0.753136000	-1.704229000
C	-4.769091000	-4.693875000	-0.877861000
H	-4.013651000	-5.479331000	-0.737856000
H	-5.385973000	-4.976314000	-1.744722000
H	-5.419127000	-4.699802000	0.009521000
C	-2.945017000	-2.990807000	-2.727279000
H	-2.457118000	-2.017776000	-2.883973000
H	-3.585119000	-3.190224000	-3.600890000
H	-2.158059000	-3.757310000	-2.714465000

TS7

Ti	0.153976000	1.543635000	0.647742000
Ti	1.474250000	-0.468975000	-0.406591000
Ti	-1.249117000	-1.125629000	0.519547000
Si	-0.588531000	4.286031000	-1.731718000
Si	4.969055000	-1.570569000	0.508459000
Si	-4.301601000	-1.669287000	-1.582410000
N	-0.437858000	0.102394000	-0.581767000
N	1.843735000	1.231009000	0.081858000
C	0.572595000	-1.457974000	1.387783000
H	0.893030000	-2.300618000	2.016480000
C	0.356713000	-0.176041000	2.016827000
C	0.640285000	-0.047357000	3.509669000
H	1.660847000	0.340767000	3.633930000
H	0.581690000	-1.014540000	4.034531000
H	-0.040474000	0.660932000	3.995740000
C	-0.482504000	3.729226000	0.077313000
C	-1.580609000	3.220306000	0.873621000
C	-1.122940000	3.026209000	2.212283000
C	0.256879000	3.426784000	2.269434000
C	0.644335000	3.878888000	0.974656000
C	3.612177000	-1.447870000	-0.811015000
C	2.650537000	-2.496274000	-1.103602000
C	1.862243000	-2.093747000	-2.218433000
C	2.307953000	-0.791871000	-2.627273000
C	3.406469000	-0.409731000	-1.795749000
C	-3.303856000	-2.076461000	-0.016316000
C	-2.339722000	-3.161882000	0.073477000
C	-1.921039000	-3.299956000	1.434948000
C	-2.605655000	-2.308467000	2.207454000
C	-3.455104000	-1.563419000	1.328759000
H	-1.096325000	0.109657000	1.833445000

C	2.560155000	-3.839612000	-0.418945000
H	3.213833000	-4.577154000	-0.911798000
H	2.863203000	-3.782400000	0.633229000
H	1.537645000	-4.238221000	-0.446135000
C	0.819551000	-2.903453000	-2.945784000
H	1.189199000	-3.203238000	-3.939734000
H	0.568970000	-3.820479000	-2.401863000
H	-0.108241000	-2.336141000	-3.102275000
C	4.204340000	0.859594000	-1.968349000
H	4.322282000	1.396155000	-1.021260000
H	5.203484000	0.641205000	-2.376392000
H	3.705046000	1.538679000	-2.669947000
C	1.752927000	-0.026573000	-3.805396000
H	1.879131000	1.056138000	-3.686613000
H	2.262829000	-0.319995000	-4.737675000
H	0.681331000	-0.222972000	-3.939124000
C	-3.182612000	-1.242783000	-3.059862000
H	-2.611460000	-2.105840000	-3.430077000
H	-3.798063000	-0.878346000	-3.897146000
H	-2.464054000	-0.453412000	-2.798349000
C	-5.491496000	-0.204679000	-1.353402000
H	-6.058687000	-0.076922000	-2.288639000
H	-6.221307000	-0.364504000	-0.548187000
H	-4.970325000	0.743167000	-1.159827000
C	-5.362878000	-3.189953000	-2.015207000
H	-5.974860000	-2.990996000	-2.908227000
H	-4.752250000	-4.079205000	-2.224898000
H	-6.047080000	-3.444209000	-1.192385000
C	-2.003250000	-4.153415000	-1.016001000
H	-2.051977000	-3.708501000	-2.015488000
H	-0.998927000	-4.574415000	-0.883677000
H	-2.713200000	-4.996008000	-0.993231000
C	-1.030726000	-4.386646000	1.982915000
H	-1.622458000	-5.280504000	2.238269000
H	-0.267552000	-4.693577000	1.257316000
H	-0.511562000	-4.065469000	2.895015000
C	-2.497988000	-2.134140000	3.702098000
H	-3.268276000	-2.725998000	4.221973000
H	-1.521545000	-2.467155000	4.075474000
H	-2.628025000	-1.086720000	4.002208000
C	-4.413746000	-0.489710000	1.790176000
H	-4.469009000	0.350961000	1.091784000
H	-5.430863000	-0.900795000	1.892029000
H	-4.122874000	-0.094937000	2.771300000
C	-1.672508000	3.115824000	-2.769391000
H	-1.543245000	3.345623000	-3.838560000
H	-1.385306000	2.066318000	-2.612425000
H	-2.743051000	3.214038000	-2.542034000
C	-1.354825000	6.030606000	-1.775311000
H	-0.740831000	6.750404000	-1.214435000
H	-1.441321000	6.398447000	-2.809217000
H	-2.361926000	6.041711000	-1.333031000
C	1.116870000	4.353034000	-2.567584000
H	0.983842000	4.523098000	-3.647435000
H	1.749902000	5.163095000	-2.181489000
H	1.663510000	3.408446000	-2.439191000
C	-3.009215000	3.020280000	0.416464000
H	-3.450695000	3.969178000	0.073668000
H	-3.090671000	2.304458000	-0.411903000
H	-3.631254000	2.650709000	1.241279000
C	2.005935000	4.443242000	0.642531000
H	2.507769000	3.858426000	-0.137740000
H	1.930798000	5.487613000	0.302976000
H	2.652889000	4.432112000	1.528677000
C	1.135115000	3.473934000	3.498858000
H	2.122591000	3.029873000	3.312946000
H	1.298489000	4.514501000	3.820753000

H	0.685260000	2.938771000	4.343730000
C	-1.986845000	2.604528000	3.378442000
H	-1.407807000	2.552205000	4.308850000
H	-2.799722000	3.328418000	3.544553000
H	-2.452485000	1.620688000	3.220195000
C	4.257439000	-1.764220000	2.264290000
H	3.625240000	-2.654828000	2.385299000
H	5.078742000	-1.839922000	2.994316000
H	3.649568000	-0.888458000	2.532435000
C	6.105657000	-0.049493000	0.563041000
H	6.611943000	0.143279000	-0.392315000
H	5.564336000	0.862031000	0.851333000
H	6.885849000	-0.224963000	1.320394000
C	6.058719000	-3.083185000	0.113669000
H	6.877885000	-3.171143000	0.843860000
H	5.492923000	-4.025132000	0.136602000
H	6.510954000	-2.993564000	-0.885043000

G

Ti	-0.058582000	1.525358000	0.765867000
Ti	1.482804000	-0.297524000	-0.430307000
Ti	-1.108598000	-1.166323000	0.675131000
Si	-0.783560000	4.236992000	-1.688347000
Si	4.988158000	-1.246566000	0.674101000
Si	-3.965893000	-1.988219000	-1.747536000
N	-0.497994000	0.108540000	-0.516819000
N	1.661906000	1.338561000	0.352788000
C	0.799149000	-1.436904000	1.228801000
H	1.199121000	-2.320649000	1.749376000
C	0.108502000	-0.370229000	2.189571000
C	1.003955000	0.105341000	3.340247000
H	1.848352000	0.686407000	2.948811000
H	1.414615000	-0.752875000	3.899321000
H	0.443780000	0.729223000	4.050116000
C	-0.902498000	3.607140000	0.096820000
C	-2.049989000	2.943314000	0.688295000
C	-1.802228000	2.759971000	2.078962000
C	-0.519520000	3.345059000	2.380243000
C	0.018973000	3.887750000	1.180194000
C	3.713000000	-1.132422000	-0.721189000
C	2.849417000	-2.179916000	-1.231326000
C	2.146389000	-1.677363000	-2.365880000
C	2.563916000	-0.317774000	-2.577300000
C	3.553956000	0.003308000	-1.599839000
C	-3.009761000	-2.354181000	-0.144266000
C	-1.922419000	-3.302193000	-0.050852000
C	-1.574290000	-3.491285000	1.325051000
C	-2.450982000	-2.674699000	2.109432000
C	-3.318391000	-1.964510000	1.215897000
H	-0.777726000	-0.860256000	2.709306000
C	2.788751000	-3.601318000	-0.723971000
H	3.761658000	-4.101884000	-0.846296000
H	2.523576000	-3.653372000	0.339294000
H	2.051301000	-4.190144000	-1.283735000
C	1.237787000	-2.430210000	-3.307686000
H	1.733895000	-2.582540000	-4.279911000
H	0.972379000	-3.419308000	-2.918766000
H	0.303966000	-1.885486000	-3.503535000
C	4.314157000	1.307756000	-1.525007000
H	4.100836000	1.846688000	-0.593928000
H	5.398879000	1.130967000	-1.585205000
H	4.045003000	1.965475000	-2.360987000
C	2.100842000	0.548359000	-3.725748000
H	2.255096000	1.614619000	-3.523412000
H	2.652792000	0.301844000	-4.647760000
H	1.033026000	0.401912000	-3.936844000
C	-2.855626000	-1.272506000	-3.112975000

H	-2.179725000	-2.023106000	-3.546551000
H	-3.476154000	-0.880965000	-3.933924000
H	-2.237360000	-0.451494000	-2.725097000
C	-5.406833000	-0.772623000	-1.498231000
H	-5.940882000	-0.679133000	-2.456760000
H	-6.135110000	-1.117891000	-0.751780000
H	-5.075447000	0.235237000	-1.213546000
C	-4.728509000	-3.628204000	-2.344661000
H	-5.310787000	-3.468876000	-3.265138000
H	-3.965547000	-4.388024000	-2.564214000
H	-5.408250000	-4.049562000	-1.589454000
C	-1.326249000	-4.097200000	-1.187216000
H	-1.428873000	-3.581046000	-2.147334000
H	-0.260294000	-4.295596000	-1.022826000
H	-1.830910000	-5.072713000	-1.276495000
C	-0.583477000	-4.491193000	1.863806000
H	-1.077556000	-5.453776000	2.074938000
H	0.224660000	-4.683960000	1.148275000
H	-0.124095000	-4.146390000	2.799659000
C	-2.505594000	-2.656468000	3.619539000
H	-3.174798000	-3.448578000	3.991641000
H	-1.516511000	-2.831551000	4.063419000
H	-2.883398000	-1.702563000	4.010257000
C	-4.451524000	-1.072366000	1.671853000
H	-4.589889000	-0.204806000	1.018357000
H	-5.401839000	-1.629400000	1.680846000
H	-4.284303000	-0.705433000	2.692237000
C	-1.551041000	3.017141000	-2.929479000
H	-1.272162000	3.311105000	-3.953375000
H	-1.186713000	1.994423000	-2.759680000
H	-2.648505000	2.998092000	-2.882578000
C	-1.728456000	5.889204000	-1.793921000
H	-1.296599000	6.640640000	-1.116659000
H	-1.693555000	6.299747000	-2.814716000
H	-2.787007000	5.768847000	-1.519984000
C	1.012934000	4.536579000	-2.231587000
H	1.033957000	4.727717000	-3.315875000
H	1.468651000	5.404490000	-1.736226000
H	1.646055000	3.661171000	-2.031091000
C	-3.313616000	2.554114000	-0.045349000
H	-3.781511000	3.432564000	-0.515091000
H	-3.122809000	1.817767000	-0.837063000
H	-4.053565000	2.126012000	0.642731000
C	1.319783000	4.653050000	1.098924000
H	1.990323000	4.240154000	0.337639000
H	1.138177000	5.713030000	0.861140000
H	1.849370000	4.617564000	2.059139000
C	0.069596000	3.502906000	3.763368000
H	1.145909000	3.285860000	3.787533000
H	-0.064473000	4.535423000	4.123738000
H	-0.421571000	2.841418000	4.488127000
C	-2.741167000	2.187425000	3.114728000
H	-2.237717000	1.465310000	3.774365000
H	-3.148429000	2.983438000	3.758473000
H	-3.592233000	1.674839000	2.651997000
C	4.572426000	-2.586113000	1.960657000
H	4.621017000	-3.605272000	1.553888000
H	5.301738000	-2.526260000	2.783682000
H	3.572647000	-2.437057000	2.391994000
C	5.153088000	0.398374000	1.615250000
H	5.748243000	1.138627000	1.063236000
H	4.167288000	0.842617000	1.811981000
H	5.653342000	0.226717000	2.581068000
C	6.675926000	-1.685543000	-0.097717000
H	7.461150000	-1.742857000	0.671804000
H	6.641477000	-2.657168000	-0.612550000
H	6.988795000	-0.933223000	-0.836676000

H			
Ti	-1.322905000	-0.983047000	-0.742656000
Ti	-0.410797000	1.388713000	0.223083000
Ti	1.600809000	-0.860102000	-0.280893000
Si	-3.525283000	-2.554463000	1.944502000
Si	-1.938955000	4.553393000	-1.099931000
Si	5.323128000	0.367365000	0.192315000
N	0.025099000	-0.450630000	0.619613000
C	-3.093440000	-2.322130000	0.113436000
C	-2.253323000	-3.235981000	-0.635347000
C	-2.295688000	-2.874569000	-2.013422000
C	-3.176831000	-1.747785000	-2.147626000
C	-3.683994000	-1.421932000	-0.857914000
C	-1.086495000	3.688806000	0.358671000
C	0.345069000	3.678372000	0.585579000
C	0.622790000	2.989614000	1.808537000
C	-0.620938000	2.519461000	2.334456000
C	-1.673959000	2.963493000	1.454574000
C	3.950828000	-0.941225000	0.162126000
C	3.688222000	-1.794839000	-0.982209000
C	2.830386000	-2.869511000	-0.578384000
C	2.574914000	-2.712523000	0.828340000
C	3.248347000	-1.539281000	1.279365000
N	-1.738632000	0.831443000	-0.809906000
H	0.346569000	1.589144000	-1.712866000
C	1.344815000	1.080103000	-1.712141000
H	2.084803000	1.769204000	-2.127717000
C	1.293412000	-0.247828000	-2.359632000
H	2.074723000	-0.421612000	-3.103680000
C	0.329248000	-1.259830000	-2.025738000
H	0.415326000	-2.144382000	-2.665724000
H	1.725028000	1.073518000	-0.532742000
C	-4.392646000	-4.239789000	2.146730000
H	-4.673943000	-4.407605000	3.197861000
H	-5.311894000	-4.284959000	1.544254000
H	-3.753473000	-5.078393000	1.837019000
C	-1.987724000	-2.515757000	3.068273000
H	-1.360188000	-1.640678000	2.848758000
H	-2.295198000	-2.466271000	4.124788000
H	-1.357875000	-3.409442000	2.954580000
C	-4.728530000	-1.245166000	2.620319000
H	-4.965657000	-1.501702000	3.664925000
H	-4.301838000	-0.232738000	2.621157000
H	-5.676805000	-1.211739000	2.066900000
C	3.225118000	-1.055024000	2.710074000
H	4.079604000	-1.458478000	3.277026000
H	3.272308000	0.036718000	2.771778000
H	2.310166000	-1.380403000	3.220713000
C	1.793450000	-3.665751000	1.698481000
H	2.474895000	-4.369809000	2.202985000
H	1.225714000	-3.139379000	2.475203000
H	1.083872000	-4.258326000	1.110858000
C	2.449957000	-4.051405000	-1.434656000
H	3.274779000	-4.781765000	-1.481709000
H	1.572306000	-4.573112000	-1.035408000
H	2.217977000	-3.750363000	-2.464668000
C	4.327632000	-1.703839000	-2.347650000
H	4.604434000	-0.675288000	-2.610881000
H	5.245039000	-2.313216000	-2.387366000
H	3.657947000	-2.082165000	-3.131678000
C	4.992509000	1.836782000	-0.973981000
H	5.866131000	2.506334000	-0.992311000
H	4.797437000	1.526431000	-2.010478000
H	4.131222000	2.430529000	-0.635557000
C	6.946738000	-0.468761000	-0.349608000
H	7.785536000	0.238975000	-0.262971000

H	7.175899000	-1.335243000	0.287952000
H	6.919272000	-0.820954000	-1.389570000
C	5.657664000	1.083649000	1.921696000
H	4.826053000	1.677100000	2.323519000
H	5.899775000	0.302251000	2.655202000
H	6.531665000	1.750210000	1.853772000
C	-1.572684000	-4.472675000	-0.099462000
H	-0.645032000	-4.693085000	-0.643767000
H	-1.323590000	-4.377872000	0.963551000
H	-2.226125000	-5.354372000	-0.206695000
C	-1.667776000	-3.640164000	-3.149728000
H	-0.748644000	-4.153294000	-2.837179000
H	-2.359672000	-4.410858000	-3.526891000
H	-1.415025000	-2.984313000	-3.993152000
C	-3.511080000	-1.034622000	-3.434915000
H	-2.739282000	-1.203140000	-4.196975000
H	-4.469691000	-1.386024000	-3.849994000
H	-3.591953000	0.049124000	-3.278627000
C	-4.689219000	-0.325891000	-0.607488000
H	-5.718115000	-0.720650000	-0.644764000
H	-4.545194000	0.148268000	0.367251000
H	-4.602340000	0.458118000	-1.369719000
C	-0.796215000	1.786141000	3.643449000
H	-0.911945000	2.496692000	4.477858000
H	-1.683417000	1.141606000	3.635625000
H	0.069765000	1.149956000	3.866147000
C	1.970219000	2.871411000	2.472892000
H	2.181019000	3.760589000	3.089803000
H	2.020665000	1.996725000	3.132892000
H	2.781896000	2.786919000	1.738607000
C	1.386904000	4.413809000	-0.228479000
H	1.084441000	4.533565000	-1.275438000
H	1.554235000	5.422790000	0.180924000
H	2.357488000	3.899116000	-0.214751000
C	-3.146370000	2.754994000	1.720700000
H	-3.612975000	3.686753000	2.077236000
H	-3.678744000	2.427516000	0.822840000
H	-3.301251000	1.998378000	2.499758000
C	-3.824835000	4.340013000	-1.105955000
H	-4.112271000	3.289691000	-1.249761000
H	-4.305294000	4.707437000	-0.189101000
H	-4.238401000	4.915944000	-1.948654000
C	-1.322346000	3.908645000	-2.782155000
H	-0.243534000	4.047259000	-2.945324000
H	-1.548140000	2.836810000	-2.876023000
H	-1.841842000	4.437889000	-3.596441000
C	-1.570045000	6.419666000	-0.973344000
H	-2.054090000	6.967143000	-1.796633000
H	-1.951253000	6.835013000	-0.028670000
H	-0.493877000	6.639587000	-1.019133000

TS8

Ti	-1.389857000	-0.926292000	-0.749748000
Ti	-0.291772000	1.379046000	0.294888000
Ti	1.483254000	-1.000590000	-0.084089000
Si	-3.914567000	-2.230769000	1.767232000
Si	-1.207350000	4.761282000	-1.132002000
Si	5.339766000	-0.127748000	-0.077617000
N	-0.140896000	-0.503197000	0.706704000
C	-3.354457000	-2.035280000	-0.034690000
C	-2.572917000	-3.028541000	-0.742627000
C	-2.478034000	-2.649717000	-2.116848000
C	-3.218222000	-1.431026000	-2.288588000
C	-3.764823000	-1.058656000	-1.026964000
C	-0.663606000	3.753110000	0.382265000
C	0.715551000	3.538171000	0.774775000
C	0.741853000	2.816223000	2.010515000

C	-0.608581000	2.534102000	2.381707000
C	-1.473244000	3.122693000	1.390629000
C	3.872137000	-1.303314000	0.174797000
C	3.410870000	-2.220378000	-0.844748000
C	2.469977000	-3.131654000	-0.268194000
C	2.349002000	-2.801705000	1.129265000
C	3.207075000	-1.688997000	1.397469000
N	-1.503036000	0.962888000	-1.008310000
H	-0.200138000	1.156051000	-1.476690000
C	1.231214000	1.000334000	-1.340859000
H	1.858010000	1.805814000	-1.728940000
C	1.256389000	-0.246720000	-2.122605000
H	2.052700000	-0.348432000	-2.866285000
C	0.291039000	-1.302167000	-1.913924000
H	0.416357000	-2.146204000	-2.600783000
H	1.778451000	0.866833000	-0.188578000
C	-4.978370000	-3.806605000	1.894652000
H	-5.347945000	-3.942012000	2.922809000
H	-5.853292000	-3.747482000	1.230627000
H	-4.417673000	-4.711844000	1.622958000
C	-2.451645000	-2.371268000	2.977627000
H	-1.728579000	-1.559092000	2.819114000
H	-2.818726000	-2.312635000	4.014505000
H	-1.905405000	-3.320026000	2.879843000
C	-4.998844000	-0.796326000	2.390044000
H	-5.321474000	-1.030482000	3.416818000
H	-4.461417000	0.161449000	2.428724000
H	-5.905103000	-0.652428000	1.786131000
C	3.401026000	-1.093630000	2.772225000
H	4.221481000	-1.602746000	3.304175000
H	3.643932000	-0.028537000	2.729627000
H	2.497297000	-1.209067000	3.384723000
C	1.522140000	-3.557476000	2.142101000
H	2.120026000	-4.351790000	2.618048000
H	1.148486000	-2.901361000	2.937564000
H	0.652854000	-4.035391000	1.674095000
C	1.908625000	-4.353071000	-0.949971000
H	2.648145000	-5.171446000	-0.949358000
H	1.013793000	-4.721767000	-0.436789000
H	1.640748000	-4.152251000	-1.995302000
C	3.899416000	-2.327461000	-2.269376000
H	4.358761000	-1.396747000	-2.622048000
H	4.653749000	-3.125507000	-2.361879000
H	3.078384000	-2.578000000	-2.955698000
C	5.029234000	1.194153000	-1.412635000
H	5.949123000	1.775507000	-1.581023000
H	4.725155000	0.773509000	-2.381140000
H	4.246265000	1.899058000	-1.099739000
C	6.835581000	-1.182924000	-0.604195000
H	7.727403000	-0.550198000	-0.731093000
H	7.070794000	-1.940661000	0.157701000
H	6.666688000	-1.710432000	-1.552976000
C	5.866759000	0.799611000	1.497327000
H	5.117121000	1.521247000	1.850375000
H	6.103002000	0.121961000	2.329152000
H	6.781326000	1.369123000	1.269229000
C	-2.061001000	-4.333270000	-0.179706000
H	-1.175725000	-4.685853000	-0.722811000
H	-1.795859000	-4.249853000	0.881002000
H	-2.827181000	-5.121185000	-0.266091000
C	-1.853021000	-3.464728000	-3.220249000
H	-1.010371000	-4.065899000	-2.854376000
H	-2.588421000	-4.161839000	-3.653649000
H	-1.481003000	-2.828886000	-4.033931000
C	-3.385661000	-0.665554000	-3.577684000
H	-2.634351000	-0.962768000	-4.320125000
H	-4.379027000	-0.843558000	-4.020160000

H	-3.280088000	0.414697000	-3.411395000
C	-4.638272000	0.155906000	-0.828818000
H	-5.697390000	-0.088543000	-1.013847000
H	-4.561036000	0.559772000	0.184381000
H	-4.350787000	0.953850000	-1.524973000
C	-1.038854000	1.837067000	3.650538000
H	-1.132320000	2.556459000	4.480332000
H	-2.009759000	1.340096000	3.536955000
H	-0.312714000	1.072705000	3.955015000
C	1.969341000	2.500320000	2.825503000
H	2.213871000	3.336684000	3.501049000
H	1.826949000	1.607468000	3.446437000
H	2.845795000	2.330126000	2.187479000
C	1.942996000	4.116513000	0.109727000
H	1.771020000	4.334840000	-0.950467000
H	2.238665000	5.060111000	0.595466000
H	2.803793000	3.436629000	0.178409000
C	-2.982538000	3.110246000	1.468659000
H	-3.364499000	4.096457000	1.775505000
H	-3.439486000	2.853591000	0.508005000
H	-3.332308000	2.384460000	2.213293000
C	-3.092237000	4.823451000	-1.352801000
H	-3.508498000	3.829475000	-1.566798000
H	-3.617171000	5.236961000	-0.481104000
H	-3.321779000	5.470835000	-2.213586000
C	-0.500776000	4.082681000	-2.763548000
H	0.597489000	4.047346000	-2.792450000
H	-0.877032000	3.066617000	-2.947092000
H	-0.827669000	4.720650000	-3.599723000
C	-0.595461000	6.549976000	-0.885684000
H	-0.897382000	7.183478000	-1.733802000
H	-1.021041000	6.991604000	0.027572000
H	0.498946000	6.610769000	-0.801538000

Complex 3

Ti	0.179197000	1.582302000	-0.838049000
Ti	1.445046000	-0.917838000	-0.793021000
Ti	-1.534119000	-0.831760000	-0.728566000
Si	-0.151028000	3.923026000	2.170759000
Si	3.570146000	-1.476756000	2.286531000
Si	-3.138358000	-1.887247000	2.505748000
N	-0.015067000	-0.096622000	0.145895000
C	0.092003000	3.648401000	0.310030000
C	-0.989040000	3.666473000	-0.657355000
C	-0.432534000	3.675536000	-1.971213000
C	0.993514000	3.663887000	-1.844972000
C	1.320363000	3.659009000	-0.455277000
C	-2.464750000	3.802780000	-0.365333000
H	-3.069447000	3.253052000	-1.097934000
H	-2.775247000	4.859677000	-0.409456000
H	-2.725552000	3.424334000	0.629206000
C	-1.184181000	3.836124000	-3.267598000
H	-2.236159000	3.541401000	-3.167882000
H	-0.742261000	3.233533000	-4.071868000
H	-1.170022000	4.889810000	-3.591480000
C	1.956052000	3.716900000	-3.004619000
H	2.965468000	3.396122000	-2.715062000
H	2.046016000	4.743758000	-3.394087000
H	1.622189000	3.077521000	-3.833111000
C	2.729583000	3.700807000	0.087357000
H	2.835580000	3.109334000	1.002103000
H	3.030507000	4.734734000	0.321334000
H	3.447999000	3.310001000	-0.644429000
C	-1.184820000	2.545112000	2.976180000
H	-2.224984000	2.545039000	2.620675000
H	-1.212671000	2.678191000	4.068840000
H	-0.761310000	1.553585000	2.763450000

C	-1.049299000	5.586424000	2.407830000
H	-0.465129000	6.414314000	1.979642000
H	-1.191850000	5.798110000	3.478746000
H	-2.039919000	5.600564000	1.932707000
C	1.477002000	4.042995000	3.145504000
H	2.036265000	3.098030000	3.166685000
H	1.231036000	4.299759000	4.188002000
H	2.144655000	4.827926000	2.764631000
C	3.168015000	-1.886603000	0.476829000
C	3.818170000	-1.261841000	-0.660210000
C	3.421671000	-1.938279000	-1.848787000
C	2.539002000	-3.004917000	-1.476699000
C	2.383137000	-2.980613000	-0.055618000
C	4.819510000	-0.133146000	-0.609833000
H	4.772006000	0.491066000	-1.512574000
H	5.846285000	-0.526683000	-0.544688000
H	4.655857000	0.521824000	0.253437000
C	3.864349000	-1.618455000	-3.254736000
H	4.191744000	-0.574905000	-3.346500000
H	3.052440000	-1.774530000	-3.977233000
H	4.710265000	-2.255061000	-3.560495000
C	2.010287000	-4.067686000	-2.406485000
H	1.002944000	-4.403603000	-2.124947000
H	2.665282000	-4.953525000	-2.388827000
H	1.968791000	-3.712793000	-3.444191000
C	1.607533000	-4.017635000	0.725003000
H	1.086111000	-3.585599000	1.584790000
H	2.279861000	-4.803909000	1.105051000
H	0.858659000	-4.508765000	0.091456000
C	2.741432000	-2.651503000	3.529600000
H	1.648423000	-2.547104000	3.554436000
H	3.115473000	-2.402734000	4.535215000
H	2.981164000	-3.707481000	3.343966000
C	5.450170000	-1.662630000	2.533145000
H	5.783732000	-2.679233000	2.277650000
H	5.716148000	-1.480054000	3.585677000
H	6.030104000	-0.959591000	1.919770000
C	3.048482000	0.289345000	2.754785000
H	3.586213000	1.054226000	2.177319000
H	3.248920000	0.476709000	3.821212000
H	1.973586000	0.433259000	2.576942000
C	-3.197628000	-1.641658000	0.626910000
C	-2.864271000	-2.686488000	-0.330577000
C	-3.276338000	-2.255392000	-1.632844000
C	-3.865372000	-0.954469000	-1.510097000
C	-3.818091000	-0.570892000	-0.138321000
C	-2.361755000	-4.078065000	-0.018146000
H	-1.752814000	-4.477128000	-0.840748000
H	-3.203375000	-4.774240000	0.132902000
H	-1.748411000	-4.099166000	0.890087000
C	-3.197193000	-3.081101000	-2.892368000
H	-3.278772000	-2.457352000	-3.791393000
H	-4.015195000	-3.818998000	-2.927609000
H	-2.252000000	-3.637780000	-2.955623000
C	-4.471286000	-0.165962000	-2.642366000
H	-3.890654000	-0.276900000	-3.568393000
H	-4.520513000	0.904510000	-2.409376000
H	-5.497381000	-0.507969000	-2.852924000
C	-4.433626000	0.690420000	0.419032000
H	-3.834385000	1.120805000	1.228289000
H	-5.437041000	0.485741000	0.826452000
H	-4.546959000	1.455037000	-0.358239000
C	-1.369961000	-2.169043000	3.145766000
H	-0.944258000	-3.119004000	2.792403000
H	-1.363021000	-2.196108000	4.246555000
H	-0.702127000	-1.360879000	2.816252000
C	-3.864755000	-0.432403000	3.490383000

H	-3.267509000	0.484805000	3.405944000
H	-3.876848000	-0.716043000	4.554618000
H	-4.898811000	-0.197221000	3.203559000
C	-4.201247000	-3.407777000	2.943128000
H	-5.238567000	-3.275980000	2.601524000
H	-4.226351000	-3.554899000	4.033962000
H	-3.820104000	-4.334993000	2.493824000
N	1.814108000	0.796890000	-1.483180000
H	2.595156000	1.193025000	-2.012315000
C	0.028734000	-1.511715000	-2.311071000
H	0.163167000	-2.353361000	-2.999611000
C	-0.933162000	-0.516249000	-2.814219000
H	-1.567876000	-0.828543000	-3.654908000
C	-1.133583000	0.775919000	-2.223126000
H	-1.927854000	1.352248000	-2.711655000
H	-0.430025000	-2.181276000	-1.348996000

TS9

Ti	0.313556000	1.438799000	-0.465827000
H	-1.511899000	1.483204000	-0.345428000
Ti	1.074431000	-1.164318000	0.206009000
Ti	-1.578668000	-0.218521000	0.431217000
Si	1.969071000	4.464032000	0.978355000
Si	3.964992000	-3.290352000	-1.048484000
Si	-5.003236000	-1.243884000	-1.159474000
N	-0.728382000	-2.001583000	0.078384000
N	0.091473000	0.415801000	1.061842000
C	-0.404003000	-0.277588000	-1.549686000
H	-0.452963000	-0.022405000	-2.615220000
C	-0.730275000	-1.630861000	-1.261308000
C	-1.113454000	-2.658836000	-2.318975000
H	-2.137039000	-3.019098000	-2.155956000
H	-0.444508000	-3.525778000	-2.244511000
H	-1.040396000	-2.241726000	-3.331487000
C	1.381350000	3.514056000	-0.556964000
C	0.068484000	3.677699000	-1.150524000
C	0.020701000	2.938267000	-2.376750000
C	1.289739000	2.307189000	-2.562085000
C	2.127768000	2.651683000	-1.454925000
C	2.960405000	-2.580782000	0.391526000
C	1.859916000	-3.257914000	1.030133000
C	1.449722000	-2.509923000	2.177154000
C	2.288688000	-1.359686000	2.280526000
C	3.212038000	-1.387770000	1.189494000
C	-3.961122000	-0.617491000	0.297499000
C	-3.449389000	-1.358800000	1.434161000
C	-2.954980000	-0.422408000	2.398458000
C	-3.146328000	0.899852000	1.880885000
C	-3.778958000	0.784575000	0.606168000
H	1.852406000	-0.022090000	-0.992760000
H	2.095585000	-0.968630000	-1.254425000
C	4.883957000	-4.837044000	-0.418590000
H	4.186354000	-5.602006000	-0.047523000
H	5.486413000	-5.295943000	-1.217439000
H	5.563495000	-4.584623000	0.408925000
C	5.272535000	-2.086666000	-1.728041000
H	5.799680000	-2.579746000	-2.559821000
H	4.823982000	-1.165244000	-2.126188000
H	6.027401000	-1.804335000	-0.981930000
C	2.897130000	-3.791512000	-2.545480000
H	2.309894000	-2.936418000	-2.909490000
H	3.551431000	-4.126002000	-3.366123000
H	2.197415000	-4.611929000	-2.334059000
C	1.231271000	-4.576722000	0.649216000
H	1.597704000	-4.944497000	-0.315359000
H	1.461531000	-5.344207000	1.405786000
H	0.138124000	-4.482623000	0.586691000

C	0.369325000	-2.946257000	3.127573000
H	-0.559021000	-3.174449000	2.586506000
H	0.671981000	-3.858117000	3.667729000
H	0.156012000	-2.174817000	3.875557000
C	2.234654000	-0.326180000	3.376498000
H	1.216392000	-0.216277000	3.768229000
H	2.894293000	-0.606464000	4.213754000
H	2.550514000	0.660586000	3.016715000
C	4.360376000	-0.421946000	1.024099000
H	5.294256000	-0.855011000	1.419606000
H	4.537835000	-0.159783000	-0.023232000
H	4.176687000	0.507345000	1.578024000
C	3.596056000	2.306560000	-1.389405000
H	4.199173000	3.109057000	-1.845872000
H	3.949014000	2.170511000	-0.364273000
H	3.809044000	1.383597000	-1.943654000
C	1.706859000	1.470970000	-3.746920000
H	2.342881000	2.051569000	-4.433847000
H	2.276579000	0.583050000	-3.440317000
H	0.838365000	1.126252000	-4.323042000
C	-1.147441000	2.885554000	-3.330395000
H	-1.080621000	3.691923000	-4.078450000
H	-1.184933000	1.935073000	-3.879132000
H	-2.102548000	3.000164000	-2.803145000
C	-1.029700000	4.595792000	-0.665205000
H	-1.019315000	4.709689000	0.425163000
H	-0.916302000	5.600875000	-1.102871000
H	-2.020530000	4.223279000	-0.953057000
C	0.911108000	4.073612000	2.512130000
H	1.345394000	4.562375000	3.398433000
H	-0.125870000	4.426521000	2.421557000
H	0.875322000	2.991697000	2.703828000
C	1.867599000	6.329017000	0.606858000
H	2.224213000	6.913707000	1.468656000
H	2.493294000	6.594445000	-0.257962000
H	0.842276000	6.657002000	0.386549000
C	3.772420000	4.093406000	1.454285000
H	3.926711000	3.050531000	1.765015000
H	4.483737000	4.317931000	0.647894000
H	4.038081000	4.729845000	2.312911000
C	-2.809271000	2.177197000	2.607614000
H	-1.905362000	2.063293000	3.218620000
H	-2.634430000	3.003439000	1.907511000
H	-3.631440000	2.477492000	3.277910000
C	-4.285154000	1.955518000	-0.201824000
H	-4.265563000	1.753491000	-1.278582000
H	-5.324870000	2.191721000	0.076084000
H	-3.683949000	2.853874000	-0.019604000
C	-4.363143000	-0.637246000	-2.848829000
H	-3.296713000	-0.858299000	-2.989634000
H	-4.919223000	-1.139453000	-3.655871000
H	-4.497372000	0.444647000	-2.987554000
C	-6.780543000	-0.596941000	-0.932371000
H	-7.432176000	-0.965664000	-1.739450000
H	-7.207550000	-0.937088000	0.022420000
H	-6.829323000	0.500912000	-0.944574000
C	-5.122865000	-3.140354000	-1.240557000
H	-5.618143000	-3.563585000	-0.356042000
H	-5.730943000	-3.411916000	-2.117609000
H	-4.150709000	-3.639518000	-1.348132000
C	-3.497344000	-2.855205000	1.628662000
H	-4.534094000	-3.203257000	1.750004000
H	-3.048086000	-3.389620000	0.783691000
H	-2.946711000	-3.150224000	2.529571000
C	-2.430433000	-0.713860000	3.783010000
H	-3.179506000	-0.424939000	4.537590000
H	-2.211724000	-1.776880000	3.925124000

H	-1.514034000	-0.147955000	3.996974000
I			
Ti	0.204988000	1.373605000	-0.464172000
H	-1.636734000	1.180931000	-0.429744000
Ti	1.214341000	-1.188476000	0.091331000
Ti	-1.546547000	-0.471141000	0.394409000
Si	1.147291000	4.686439000	1.102048000
Si	4.680134000	-2.413922000	-0.966015000
Si	-4.932953000	-1.510465000	-1.229129000
N	-0.539859000	-2.158796000	0.011494000
N	0.028317000	0.326881000	1.043199000
C	-0.359592000	-0.398791000	-1.596961000
H	-0.436143000	-0.128426000	-2.656258000
C	-0.625092000	-1.758643000	-1.315900000
C	-0.929508000	-2.792485000	-2.391572000
H	-1.386002000	-2.338948000	-3.280428000
H	-1.586561000	-3.576033000	-1.997249000
H	0.014165000	-3.267612000	-2.696448000
C	0.774876000	3.652011000	-0.447650000
C	-0.461790000	3.529961000	-1.188298000
C	-0.203020000	2.811227000	-2.406192000
C	1.181775000	2.471636000	-2.436089000
C	1.783890000	2.976524000	-1.237727000
C	3.345537000	-2.199279000	0.360361000
C	2.338659000	-3.165970000	0.725365000
C	1.666377000	-2.723206000	1.908360000
C	2.211118000	-1.456634000	2.272112000
C	3.234587000	-1.127247000	1.322570000
C	-3.903459000	-0.982087000	0.275463000
C	-3.328766000	-1.807053000	1.319515000
C	-2.848852000	-0.950985000	2.359671000
C	-3.117410000	0.407980000	1.986505000
C	-3.784565000	0.390185000	0.724931000
H	1.759148000	0.418103000	-0.642737000
H	2.075735000	-1.289825000	-1.403092000
C	6.181131000	-3.240120000	-0.126467000
H	5.916075000	-4.220096000	0.297649000
H	7.001897000	-3.398905000	-0.842740000
H	6.572740000	-2.622470000	0.695517000
C	5.265562000	-0.773473000	-1.730514000
H	5.878465000	-0.987852000	-2.619851000
H	4.409235000	-0.165905000	-2.052804000
H	5.881597000	-0.173013000	-1.047199000
C	4.139698000	-3.520647000	-2.415588000
H	3.201001000	-3.163020000	-2.861646000
H	4.915995000	-3.485610000	-3.196048000
H	4.009800000	-4.573370000	-2.130894000
C	2.023789000	-4.466584000	0.023064000
H	1.936593000	-4.334470000	-1.062201000
H	2.810099000	-5.217906000	0.201836000
H	1.074890000	-4.879611000	0.385350000
C	0.618349000	-3.517784000	2.639384000
H	-0.259117000	-3.688589000	1.999972000
H	1.016965000	-4.498493000	2.941200000
H	0.289939000	-3.002234000	3.548978000
C	1.865307000	-0.635382000	3.487970000
H	1.016017000	-1.066421000	4.030906000
H	2.718191000	-0.591360000	4.183491000
H	1.593240000	0.391668000	3.213699000
C	4.141036000	0.073658000	1.459470000
H	5.068242000	-0.196203000	1.992647000
H	4.424572000	0.490332000	0.488664000
H	3.652405000	0.867927000	2.037282000
C	3.269620000	2.937179000	-0.971531000
H	3.768361000	3.781720000	-1.474633000
H	3.500394000	3.005594000	0.097092000

H	3.717265000	2.012195000	-1.352842000
C	1.912874000	1.714407000	-3.517355000
H	2.707402000	2.333531000	-3.960906000
H	2.377633000	0.801598000	-3.118522000
H	1.236247000	1.417503000	-4.328204000
C	-1.223053000	2.526401000	-3.481684000
H	-1.414187000	3.426366000	-4.087296000
H	-0.880976000	1.739867000	-4.165945000
H	-2.181724000	2.201921000	-3.056933000
C	-1.786841000	4.184637000	-0.874581000
H	-2.030748000	4.147272000	0.191987000
H	-1.772414000	5.245572000	-1.172449000
H	-2.602204000	3.700109000	-1.424032000
C	-0.400515000	5.498662000	1.851438000
H	-0.082462000	6.117932000	2.704734000
H	-0.926727000	6.157452000	1.147575000
H	-1.120994000	4.763397000	2.237157000
C	2.334421000	6.086784000	0.599274000
H	2.562359000	6.729992000	1.462894000
H	3.288241000	5.703045000	0.211310000
H	1.890657000	6.721567000	-0.181686000
C	1.937478000	3.656838000	2.490857000
H	1.294198000	2.808517000	2.764152000
H	2.922777000	3.252504000	2.221643000
H	2.073471000	4.281805000	3.387306000
C	-2.816846000	1.618190000	2.834896000
H	-3.614062000	1.788890000	3.576653000
H	-1.872358000	1.497800000	3.380434000
H	-2.733941000	2.526413000	2.224861000
C	-4.402059000	1.601027000	0.068068000
H	-4.382959000	1.534628000	-1.025487000
H	-5.454083000	1.704504000	0.378650000
H	-3.883406000	2.521657000	0.356022000
C	-2.264083000	-1.361136000	3.687802000
H	-1.404463000	-0.736065000	3.960952000
H	-3.018916000	-1.250038000	4.482959000
H	-1.937329000	-2.405687000	3.686677000
C	-3.302261000	-3.315490000	1.364974000
H	-4.310879000	-3.718343000	1.545772000
H	-2.922295000	-3.746528000	0.432611000
H	-2.655506000	-3.672296000	2.174442000
C	-4.915165000	-3.385985000	-1.537388000
H	-5.317074000	-3.956826000	-0.689632000
H	-5.554409000	-3.598279000	-2.408634000
H	-3.914448000	-3.777178000	-1.763585000
C	-4.358082000	-0.669933000	-2.839931000
H	-4.594169000	0.403113000	-2.867309000
H	-3.274463000	-0.774542000	-2.988123000
H	-4.861526000	-1.134828000	-3.701852000
C	-6.746320000	-1.023289000	-0.909035000
H	-6.872407000	0.061735000	-0.788437000
H	-7.384766000	-1.338917000	-1.748466000
H	-7.131403000	-1.504952000	0.001679000

TS10

Ti	0.270774000	1.363697000	-0.459009000
H	-1.509603000	0.945693000	-0.808159000
Ti	1.178737000	-1.123921000	0.257694000
Ti	-1.620684000	-0.472924000	0.410430000
Si	1.074394000	4.701121000	1.066833000
Si	4.532044000	-2.488281000	-1.048419000
Si	-4.918408000	-1.498209000	-1.327907000
N	-0.585551000	-2.081435000	0.279670000
N	-0.104024000	0.454210000	1.075890000
C	0.194050000	-0.643984000	-1.551132000
H	0.190029000	-0.472755000	-2.630972000
C	-0.570238000	-1.805420000	-1.113609000

C	-0.841586000	-2.951263000	-2.079084000
H	-1.159727000	-2.577957000	-3.062654000
H	-1.618410000	-3.613495000	-1.679034000
H	0.069647000	-3.553857000	-2.228120000
C	0.817678000	3.642889000	-0.489629000
C	-0.367274000	3.478635000	-1.304437000
C	-0.023520000	2.723632000	-2.476348000
C	1.366237000	2.404822000	-2.406108000
C	1.885821000	2.963317000	-1.193955000
C	3.307339000	-2.162746000	0.363004000
C	2.320588000	-3.118223000	0.812313000
C	1.731181000	-2.657556000	2.030471000
C	2.321392000	-1.396712000	2.350311000
C	3.290964000	-1.090514000	1.336966000
C	-3.974646000	-0.943861000	0.220280000
C	-3.445673000	-1.742739000	1.305950000
C	-2.977885000	-0.860735000	2.328570000
C	-3.234307000	0.491564000	1.914734000
C	-3.854853000	0.442285000	0.633596000
H	1.864539000	0.554173000	-0.216949000
H	1.679837000	-1.000085000	-1.437224000
C	5.586101000	-3.991545000	-0.537914000
H	6.334734000	-4.229653000	-1.308906000
H	6.124248000	-3.796903000	0.401570000
H	4.971492000	-4.890154000	-0.383790000
C	3.712904000	-2.868743000	-2.725180000
H	3.137209000	-2.004676000	-3.084901000
H	4.493778000	-3.090731000	-3.469876000
H	3.031561000	-3.730292000	-2.699771000
C	5.726855000	-1.043372000	-1.370605000
H	6.414332000	-1.335745000	-2.179742000
H	5.206768000	-0.132316000	-1.699411000
H	6.339790000	-0.789636000	-0.495186000
C	4.230007000	0.089096000	1.422334000
H	5.150810000	-0.189818000	1.961281000
H	4.518664000	0.460908000	0.436487000
H	3.768206000	0.917922000	1.972668000
C	1.962154000	-4.444283000	0.184180000
H	2.326243000	-4.526493000	-0.845886000
H	2.402986000	-5.275499000	0.758332000
H	0.873165000	-4.590906000	0.174986000
C	0.725136000	-3.433920000	2.836304000
H	-0.148805000	-3.689988000	2.221588000
H	1.168528000	-4.371084000	3.208664000
H	0.379915000	-2.863080000	3.706214000
C	2.040669000	-0.563857000	3.576271000
H	1.065856000	-0.812942000	4.011539000
H	2.808004000	-0.733305000	4.349005000
H	2.029793000	0.507298000	3.342397000
C	-3.416958000	-3.248994000	1.395360000
H	-4.415679000	-3.647099000	1.635322000
H	-3.083581000	-3.709012000	0.459282000
H	-2.730085000	-3.581126000	2.182311000
C	-2.392340000	-1.246356000	3.664470000
H	-3.167833000	-1.219181000	4.447255000
H	-1.973531000	-2.258368000	3.649270000
H	-1.595027000	-0.554780000	3.966130000
C	-2.950422000	1.720898000	2.741140000
H	-3.734460000	1.876624000	3.499994000
H	-1.989064000	1.637469000	3.264181000
H	-2.911509000	2.623609000	2.118756000
C	-4.420850000	1.639143000	-0.091990000
H	-4.375129000	1.521857000	-1.180690000
H	-5.477118000	1.788301000	0.183801000
H	-3.883543000	2.558028000	0.166677000
C	-4.175458000	-0.778741000	-2.928019000
H	-4.676264000	-1.216698000	-3.805642000

H	-4.290622000	0.312095000	-2.997257000
H	-3.102282000	-1.001989000	-3.004066000
C	-6.724438000	-0.908941000	-1.179239000
H	-7.311279000	-1.243224000	-2.048691000
H	-7.201840000	-1.320032000	-0.277590000
H	-6.806201000	0.185598000	-1.127218000
C	-4.983838000	-3.386917000	-1.541042000
H	-3.997593000	-3.836158000	-1.719421000
H	-5.435550000	-3.894008000	-0.677710000
H	-5.609003000	-3.613105000	-2.419078000
C	3.354784000	2.977283000	-0.846244000
H	3.850516000	3.836767000	-1.326272000
H	3.525568000	3.055608000	0.232640000
H	3.855116000	2.067725000	-1.199495000
C	1.789919000	3.690897000	2.510267000
H	2.804248000	3.316856000	2.312869000
H	1.842245000	4.315861000	3.415493000
H	1.152019000	2.823357000	2.730912000
C	2.270920000	6.116404000	0.629791000
H	1.868700000	6.738526000	-0.183266000
H	2.431702000	6.769478000	1.501152000
H	3.254430000	5.746632000	0.307903000
C	-0.528614000	5.499227000	1.706743000
H	-0.273564000	6.137641000	2.567092000
H	-1.020545000	6.137565000	0.960359000
H	-1.259409000	4.758023000	2.059833000
C	-1.723804000	4.103229000	-1.078479000
H	-2.016875000	4.091605000	-0.023786000
H	-1.724908000	5.154515000	-1.409255000
H	-2.498142000	3.577587000	-1.648900000
C	-0.962532000	2.374702000	-3.605327000
H	-1.970993000	2.149932000	-3.237704000
H	-1.043181000	3.209406000	-4.319878000
H	-0.613768000	1.497807000	-4.165863000
C	2.178209000	1.643343000	-3.424020000
H	2.891428000	2.307185000	-3.936996000
H	2.757161000	0.835815000	-2.953014000
H	1.540244000	1.192009000	-4.194256000

J

Ti	0.689216000	1.186811000	-0.638973000
H	-1.231526000	1.267537000	-0.949426000
Ti	0.638084000	-1.342150000	0.107211000
Ti	-1.818059000	0.054063000	0.344935000
Si	2.573237000	3.855886000	1.243662000
Si	4.124507000	-2.903101000	-0.405336000
Si	-5.091296000	-0.836585000	-1.133987000
N	-1.372582000	-1.459507000	-0.599249000
N	-0.037377000	0.432387000	0.891010000
C	0.321596000	-0.661432000	-2.077168000
H	-0.325216000	0.109959000	-2.539566000
C	-0.504298000	-1.829883000	-1.602377000
C	-0.761688000	-3.029052000	-2.493769000
H	-1.452614000	-2.751380000	-3.308622000
H	-1.225573000	-3.849777000	-1.932824000
H	0.162349000	-3.396475000	-2.960962000
C	1.983409000	3.119008000	-0.410082000
C	0.754705000	3.504278000	-1.074174000
C	0.713161000	2.900333000	-2.368669000
C	1.915261000	2.141068000	-2.539038000
C	2.696314000	2.270713000	-1.343328000
C	2.504005000	-2.721693000	0.558900000
C	1.370308000	-3.606166000	0.381295000
C	0.420288000	-3.350295000	1.417637000
C	0.962017000	-2.333079000	2.272989000
C	2.227555000	-1.937645000	1.750432000
C	-4.165565000	0.042319000	0.264231000

C	-3.782106000	-0.480244000	1.560386000
C	-3.186254000	0.578427000	2.322491000
C	-3.197944000	1.763945000	1.527299000
C	-3.782297000	1.441944000	0.262622000
H	1.147341000	-0.920784000	-2.753090000
H	1.966604000	-0.046357000	-0.284027000
C	4.764912000	-4.685641000	-0.190397000
H	5.749923000	-4.792778000	-0.670656000
H	4.885809000	-4.936530000	0.873792000
H	4.098738000	-5.437158000	-0.634791000
C	5.522503000	-1.778475000	0.224210000
H	6.443116000	-2.033159000	-0.324063000
H	5.328884000	-0.711046000	0.058815000
H	5.727666000	-1.925732000	1.293625000
C	3.902966000	-2.560316000	-2.264822000
H	3.559263000	-1.530389000	-2.434997000
H	4.858993000	-2.689684000	-2.795431000
H	3.172121000	-3.233160000	-2.735725000
C	1.281823000	-4.777787000	-0.566430000
H	1.785678000	-4.586968000	-1.521626000
H	1.756682000	-5.663607000	-0.114407000
H	0.241391000	-5.044484000	-0.783241000
C	-0.872673000	-4.101583000	1.610033000
H	-1.443336000	-4.162763000	0.674111000
H	-0.680943000	-5.129270000	1.958578000
H	-1.513934000	-3.612820000	2.351858000
C	0.332324000	-1.795181000	3.532740000
H	-0.738197000	-2.028003000	3.575831000
H	0.804693000	-2.241611000	4.422645000
H	0.438616000	-0.705899000	3.603941000
C	3.114801000	-0.905242000	2.402363000
H	3.787994000	-1.371296000	3.140878000
H	3.733256000	-0.381323000	1.667710000
H	2.513984000	-0.153809000	2.930434000
C	-4.056450000	-1.870505000	2.088476000
H	-5.131028000	-2.003815000	2.291733000
H	-3.750638000	-2.649492000	1.382895000
H	-3.525420000	-2.045512000	3.032765000
C	-2.718452000	0.526426000	3.756760000
H	-3.457512000	1.004606000	4.420018000
H	-2.580640000	-0.501847000	4.110081000
H	-1.766112000	1.056644000	3.891109000
C	-2.753086000	3.118701000	2.015811000
H	-3.485065000	3.535220000	2.727164000
H	-1.787541000	3.064494000	2.536158000
H	-2.652902000	3.836948000	1.194360000
C	-4.097022000	2.445694000	-0.823817000
H	-3.902027000	2.046127000	-1.824895000
H	-5.157551000	2.742322000	-0.782980000
H	-3.499198000	3.358286000	-0.709428000
C	-5.095748000	-2.728148000	-0.951707000
H	-4.072455000	-3.127184000	-0.915929000
H	-5.635422000	-3.077034000	-0.060985000
H	-5.594450000	-3.165530000	-1.830862000
C	-4.343130000	-0.467174000	-2.848702000
H	-4.582640000	0.539106000	-3.219620000
H	-3.249556000	-0.577151000	-2.837267000
H	-4.742864000	-1.185413000	-3.581766000
C	-6.901202000	-0.237423000	-1.128825000
H	-7.477553000	-0.712374000	-1.937695000
H	-7.398665000	-0.479533000	-0.178047000
H	-6.970295000	0.851429000	-1.268210000
C	4.095945000	1.726105000	-1.190631000
H	4.838104000	2.483373000	-1.491508000
H	4.312051000	1.438118000	-0.158702000
H	4.250149000	0.844516000	-1.823475000
C	2.325519000	1.433083000	-3.805394000

H	2.820003000	2.133957000	-4.497002000
H	3.028927000	0.615307000	-3.608030000
H	1.460616000	1.009290000	-4.332713000
C	-0.365374000	3.095984000	-3.406024000
H	-0.136348000	3.965379000	-4.043495000
H	-0.458175000	2.222766000	-4.064576000
H	-1.343412000	3.269799000	-2.942004000
C	-0.283058000	4.470932000	-0.557756000
H	-0.280164000	4.529514000	0.535672000
H	-0.088929000	5.483133000	-0.947708000
H	-1.292220000	4.183354000	-0.877266000
C	1.370207000	3.496224000	2.671090000
H	1.843535000	3.755926000	3.630886000
H	0.440088000	4.077235000	2.599352000
H	1.095896000	2.432480000	2.695360000
C	2.728985000	5.739253000	1.007306000
H	3.083297000	6.215068000	1.934502000
H	3.449417000	5.981662000	0.212289000
H	1.771427000	6.207902000	0.740657000
C	4.280695000	3.221604000	1.786615000
H	4.281340000	2.148521000	2.022299000
H	5.067754000	3.411695000	1.044462000
H	4.562817000	3.756113000	2.707321000

TS11

Ti	-0.532159000	1.352542000	0.703894000
H	1.391401000	1.235512000	0.774932000
Ti	-0.930925000	-1.308281000	0.061398000
Ti	1.659592000	-0.202968000	-0.348477000
Si	-1.559483000	4.377209000	-1.333983000
Si	-4.544271000	-2.732762000	0.119887000
Si	4.935370000	-1.399673000	1.061997000
N	1.058113000	-1.582051000	0.743912000
N	-0.065667000	0.373559000	-0.810438000
C	-0.092483000	-0.151430000	2.350373000
H	0.803473000	0.351628000	2.751526000
C	0.277823000	-1.575652000	1.911901000
C	0.578259000	-2.626520000	2.985891000
H	1.514166000	-2.360297000	3.499476000
H	0.702999000	-3.621013000	2.539819000
H	-0.221880000	-2.669985000	3.737964000
C	-1.356241000	3.505113000	0.342385000
C	-0.294002000	3.623897000	1.324057000
C	-0.714404000	2.986736000	2.537950000
C	-2.021657000	2.452698000	2.328881000
C	-2.415553000	2.757969000	0.987301000
C	-2.792760000	-2.620523000	-0.605418000
C	-1.714189000	-3.538197000	-0.280065000
C	-0.652452000	-3.363825000	-1.216238000
C	-1.019652000	-2.307863000	-2.103612000
C	-2.329898000	-1.849213000	-1.732441000
C	4.018078000	-0.443784000	-0.291095000
C	3.577739000	-0.942403000	-1.578133000
C	3.087969000	0.160997000	-2.354675000
C	3.209400000	1.344584000	-1.570099000
C	3.772457000	0.983740000	-0.305437000
H	-0.881518000	-0.168545000	3.118638000
H	-1.930386000	0.187873000	0.619652000
H	-1.106867000	-1.907304000	1.705610000
H	-2.108701000	-1.501988000	1.336432000
C	-5.236957000	-4.440288000	-0.366705000
H	-6.276661000	-4.550025000	-0.022205000
H	-5.231573000	-4.575031000	-1.458379000
H	-4.656501000	-5.265112000	0.070392000
C	-5.739961000	-1.432924000	-0.586152000
H	-6.739724000	-1.618547000	-0.163118000
H	-5.459113000	-0.404676000	-0.319403000

H	-5.831593000	-1.487093000	-1.679420000
C	-4.630479000	-2.567592000	2.013610000
H	-4.304607000	-1.570953000	2.341558000
H	-5.672340000	-2.708893000	2.342370000
H	-4.016149000	-3.306817000	2.545398000
C	-1.740272000	-4.621885000	0.772507000
H	-2.294104000	-4.313704000	1.667456000
H	-2.219984000	-5.534621000	0.383339000
H	-0.725098000	-4.897002000	1.085002000
C	0.601220000	-4.198407000	-1.251948000
H	1.215325000	-4.032645000	-0.355527000
H	0.350906000	-5.268655000	-1.306668000
H	1.216123000	-3.957275000	-2.126229000
C	-0.246909000	-1.825800000	-3.301799000
H	0.797486000	-2.156017000	-3.257869000
H	-0.682473000	-2.219909000	-4.234387000
H	-0.246797000	-0.730870000	-3.361894000
C	-3.072543000	-0.769108000	-2.484248000
H	-3.713504000	-1.204148000	-3.268759000
H	-3.710239000	-0.173649000	-1.823563000
H	-2.368430000	-0.085088000	-2.972205000
C	3.768170000	-2.347814000	-2.102871000
H	4.831802000	-2.535761000	-2.320785000
H	3.437525000	-3.107839000	-1.388145000
H	3.216400000	-2.503168000	-3.038783000
C	2.664422000	0.155123000	-3.803645000
H	3.452785000	0.605415000	-4.428418000
H	2.487015000	-0.857094000	-4.183480000
H	1.748609000	0.739903000	-3.964566000
C	2.865258000	2.724970000	-2.066885000
H	3.594063000	3.062949000	-2.821574000
H	1.873056000	2.748607000	-2.538308000
H	2.870087000	3.462005000	-1.255999000
C	4.178315000	1.964587000	0.771982000
H	3.821222000	1.663970000	1.762946000
H	5.275433000	2.051061000	0.822086000
H	3.778234000	2.964229000	0.567051000
C	4.531404000	-3.257054000	1.064155000
H	3.445412000	-3.424444000	1.078458000
H	4.954812000	-3.791630000	0.202972000
H	4.954473000	-3.713860000	1.972449000
C	4.534496000	-0.753820000	2.809214000
H	5.012588000	0.210487000	3.028791000
H	3.451969000	-0.641893000	2.965263000
H	4.903183000	-1.476828000	3.553494000
C	6.807721000	-1.190393000	0.771362000
H	7.390382000	-1.719392000	1.541162000
H	7.108637000	-1.591065000	-0.207919000
H	7.104961000	-0.131597000	0.798558000
C	-3.781195000	2.444937000	0.421522000
H	-4.504657000	3.228599000	0.698814000
H	-3.765885000	2.378196000	-0.672462000
H	-4.159167000	1.490765000	0.809037000
C	-2.881072000	1.736621000	3.339226000
H	-3.702370000	2.386510000	3.680715000
H	-3.330627000	0.830184000	2.911531000
H	-2.305577000	1.440599000	4.224508000
C	0.068119000	2.939735000	3.826930000
H	-0.119555000	3.841937000	4.430781000
H	-0.208192000	2.070552000	4.436858000
H	1.149162000	2.886662000	3.643778000
C	0.986142000	4.416523000	1.195520000
H	1.385834000	4.391107000	0.177883000
H	0.815933000	5.473317000	1.458371000
H	1.759843000	4.030548000	1.870305000
C	-0.101986000	5.520034000	-1.766702000
H	-0.362635000	6.071682000	-2.683598000

H	0.097875000	6.264411000	-0.983582000
H	0.831561000	4.978542000	-1.968735000
C	-3.093607000	5.501549000	-1.224544000
H	-3.217414000	6.067775000	-2.160515000
H	-4.021347000	4.938521000	-1.054823000
H	-2.992726000	6.229950000	-0.406446000
C	-1.780901000	3.156597000	-2.773667000
H	-0.964492000	2.421602000	-2.795266000
H	-2.722407000	2.593879000	-2.704997000
H	-1.789263000	3.698158000	-3.732543000

K

Ti	-0.239993000	1.299729000	0.754089000
H	1.374394000	1.073178000	-0.222790000
Ti	-1.239710000	-0.904676000	-0.643533000
Ti	1.503227000	-0.745134000	-0.661210000
Si	-0.646179000	3.704085000	-2.122263000
Si	-4.636598000	-1.483777000	1.461263000
Si	4.901701000	-0.701211000	1.583937000
N	0.191554000	-0.943978000	0.754087000
N	0.168847000	-0.979406000	-1.815650000
C	-0.015697000	0.415891000	2.677860000
H	1.031431000	0.726280000	2.879985000
C	-0.042565000	-1.039851000	2.223531000
C	0.960831000	-1.979644000	2.904456000
H	1.984990000	-1.611826000	2.757697000
H	0.895484000	-2.998945000	2.496573000
H	0.759186000	-2.022508000	3.985087000
C	-0.636158000	3.371975000	-0.249905000
C	0.522097000	3.522237000	0.599222000
C	0.120752000	3.349846000	1.962220000
C	-1.289147000	3.110211000	1.981310000
C	-1.756275000	3.116743000	0.634150000
C	-3.454901000	-1.793282000	0.008265000
C	-2.495524000	-2.871833000	-0.023996000
C	-2.034721000	-3.043445000	-1.370080000
C	-2.679089000	-2.065334000	-2.186341000
C	-3.532758000	-1.279843000	-1.344987000
C	3.875098000	-1.058578000	0.030830000
C	3.324385000	-2.315807000	-0.424205000
C	2.999130000	-2.202013000	-1.818007000
C	3.313892000	-0.872593000	-2.239511000
C	3.832640000	-0.165999000	-1.109744000
H	-0.630398000	0.636706000	3.558297000
H	-1.073991000	0.915591000	-0.861497000
H	-1.055951000	-1.437027000	2.376531000
H	-1.799528000	0.399090000	0.850766000
C	-5.623588000	-3.093498000	1.723016000
H	-4.976186000	-3.942259000	1.984375000
H	-6.354171000	-2.971263000	2.537499000
H	-6.179947000	-3.369596000	0.815129000
C	-5.919464000	-0.120635000	1.124020000
H	-6.601621000	-0.073000000	1.987377000
H	-5.472442000	0.875420000	1.006101000
H	-6.531819000	-0.325210000	0.235265000
C	-3.774076000	-1.033413000	3.095673000
H	-3.079258000	-0.194366000	2.956395000
H	-4.530159000	-0.734897000	3.838979000
H	-3.206797000	-1.868946000	3.529898000
C	-4.464376000	-0.207463000	-1.863303000
H	-5.448182000	-0.634367000	-2.117773000
H	-4.629485000	0.587271000	-1.130283000
H	-4.070100000	0.254180000	-2.777712000
C	-2.485835000	-1.910407000	-3.674391000
H	-3.142619000	-2.600348000	-4.228752000
H	-2.718391000	-0.892529000	-4.012053000
H	-1.448025000	-2.122903000	-3.958954000

C	-1.096452000	-4.116550000	-1.856723000
H	-1.659157000	-5.006984000	-2.182089000
H	-0.499120000	-3.765562000	-2.705810000
H	-0.404469000	-4.436398000	-1.066824000
C	-2.136026000	-3.802554000	1.111948000
H	-2.360541000	-3.361924000	2.089884000
H	-2.701726000	-4.744966000	1.035234000
H	-1.069035000	-4.062267000	1.102203000
C	-2.147875000	2.974152000	3.211617000
H	-2.644932000	3.930769000	3.439558000
H	-2.930045000	2.216450000	3.080988000
H	-1.553957000	2.694605000	4.089824000
C	-3.208571000	2.998496000	0.246652000
H	-3.638880000	3.993666000	0.049317000
H	-3.340801000	2.390017000	-0.651763000
H	-3.790483000	2.542047000	1.055719000
C	1.008346000	3.511916000	3.170476000
H	1.045898000	4.569101000	3.478951000
H	0.641412000	2.930558000	4.025211000
H	2.038839000	3.194182000	2.966855000
C	1.908958000	3.944257000	0.174248000
H	2.110883000	3.685128000	-0.869410000
H	2.023916000	5.035057000	0.281841000
H	2.684680000	3.471933000	0.789935000
C	-2.335810000	3.395772000	-2.934972000
H	-3.142150000	4.010889000	-2.513633000
H	-2.252341000	3.648239000	-4.003701000
H	-2.635342000	2.341043000	-2.869662000
C	-0.230448000	5.549679000	-2.358762000
H	0.760617000	5.804818000	-1.956913000
H	-0.232364000	5.814671000	-3.427156000
H	-0.966783000	6.193029000	-1.854600000
C	0.611732000	2.653318000	-3.078421000
H	1.654186000	2.888934000	-2.822764000
H	0.449834000	1.583282000	-2.888302000
H	0.491621000	2.833838000	-4.158613000
C	3.221444000	-3.610456000	0.351454000
H	4.135873000	-4.212934000	0.227105000
H	3.077999000	-3.439794000	1.421757000
H	2.382347000	-4.222767000	-0.005237000
C	2.519231000	-3.303803000	-2.728746000
H	3.366024000	-3.738578000	-3.284687000
H	2.041266000	-4.117495000	-2.170840000
H	1.794151000	-2.926092000	-3.460402000
C	3.163117000	-0.345777000	-3.645733000
H	4.027201000	-0.635607000	-4.265725000
H	2.258017000	-0.741783000	-4.123707000
H	3.096687000	0.748674000	-3.664316000
C	4.380869000	1.241271000	-1.177128000
H	4.416417000	1.713954000	-0.189623000
H	5.403477000	1.240799000	-1.587121000
H	3.770283000	1.880222000	-1.827536000
C	4.263763000	0.764327000	2.618448000
H	4.968602000	0.977933000	3.437063000
H	4.156691000	1.684730000	2.027560000
H	3.286877000	0.544593000	3.070600000
C	6.675785000	-0.297677000	1.015888000
H	6.728140000	0.609988000	0.399445000
H	7.330338000	-0.143476000	1.887621000
H	7.097612000	-1.123928000	0.424884000
C	5.061706000	-2.188878000	2.760357000
H	4.118924000	-2.473386000	3.246727000
H	5.466000000	-3.078071000	2.257155000
H	5.769149000	-1.915312000	3.558948000

TS12

Ti	-0.005172000	1.374424000	-0.746025000
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H	-1.563397000	0.770809000	0.224568000
Ti	1.395378000	-0.714972000	0.696881000
Ti	-1.328139000	-1.015709000	0.569597000
Si	0.152037000	3.670072000	2.183280000
Si	4.590311000	-1.334801000	-1.699635000
Si	-4.930093000	-0.769474000	-1.272886000
N	0.066949000	-0.875370000	-0.801763000
N	-0.013453000	-1.031613000	1.786740000
C	0.416932000	0.468990000	-2.718180000
H	-0.640671000	0.750746000	-2.945799000
C	0.469027000	-0.975972000	-2.233765000
C	-0.381488000	-1.961733000	-3.038390000
H	-1.435858000	-1.662251000	-3.025282000
H	-0.300185000	-2.973048000	-2.617820000
H	-0.040635000	-1.991284000	-4.084156000
C	0.052675000	3.392450000	0.308594000
C	-1.189566000	3.346837000	-0.443106000
C	-0.878236000	3.338435000	-1.838462000
C	0.541464000	3.398454000	-1.979155000
C	1.125782000	3.419596000	-0.675992000
C	3.598448000	-1.455300000	-0.088357000
C	2.846188000	-2.587458000	0.411575000
C	2.640629000	-2.422604000	1.821864000
C	3.223536000	-1.176827000	2.207342000
C	3.805842000	-0.577963000	1.046006000
C	-3.731601000	-1.427638000	0.038320000
C	-3.012408000	-2.671086000	-0.081159000
C	-2.460112000	-3.012070000	1.197887000
C	-2.851022000	-2.001123000	2.135431000
C	-3.598931000	-1.013645000	1.423054000
H	1.016428000	0.693658000	-3.606863000
H	1.305248000	1.086881000	0.554310000
H	1.518790000	-1.309082000	-2.266471000
H	1.374781000	0.961280000	-1.733956000
C	4.497772000	0.369286000	-2.545688000
H	5.117593000	1.122011000	-2.038841000
H	4.864207000	0.288663000	-3.581003000
H	3.468748000	0.752896000	-2.575356000
C	6.412274000	-1.678678000	-1.258235000
H	6.531559000	-2.676978000	-0.812304000
H	7.047115000	-1.635181000	-2.156626000
H	6.806398000	-0.946765000	-0.538936000
C	4.107262000	-2.632036000	-3.008650000
H	3.077949000	-2.526701000	-3.379285000
H	4.777287000	-2.503632000	-3.873398000
H	4.233103000	-3.662334000	-2.649497000
C	4.639736000	0.681373000	1.057256000
H	5.702862000	0.441420000	1.221908000
H	4.560659000	1.229649000	0.113144000
H	4.335508000	1.360561000	1.863406000
C	3.225790000	-0.624736000	3.612435000
H	4.037329000	-1.073940000	4.207674000
H	3.374559000	0.462184000	3.624595000
H	2.278846000	-0.839597000	4.124772000
C	1.982198000	-3.389443000	2.772268000
H	2.735211000	-3.872166000	3.415672000
H	1.258170000	-2.876322000	3.419131000
H	1.448649000	-4.183483000	2.237260000
C	2.415624000	-3.808756000	-0.370825000
H	2.113346000	-3.557303000	-1.393437000
H	3.233084000	-4.544639000	-0.438470000
H	1.567299000	-4.308679000	0.113297000
C	-1.724441000	-4.286772000	1.532424000
H	-2.435122000	-5.089989000	1.788101000
H	-1.120958000	-4.644480000	0.687376000
H	-1.056046000	-4.147698000	2.389830000
C	-2.536122000	-2.012996000	3.610571000

H	-1.531061000	-2.411329000	3.796226000
H	-2.571586000	-1.004978000	4.041134000
H	-3.260555000	-2.636172000	4.159637000
C	-4.217844000	0.203462000	2.072350000
H	-4.226007000	1.066323000	1.399888000
H	-5.258062000	0.001818000	2.375331000
H	-3.666871000	0.490115000	2.976658000
C	-2.999820000	-3.605220000	-1.269717000
H	-3.782069000	-4.373284000	-1.156001000
H	-3.187128000	-3.080378000	-2.212844000
H	-2.042908000	-4.134413000	-1.366562000
C	-4.097405000	-0.361263000	-2.936459000
H	-3.731137000	-1.253994000	-3.462664000
H	-4.820643000	0.133465000	-3.603489000
H	-3.244802000	0.319769000	-2.804601000
C	-5.875626000	0.790831000	-0.735437000
H	-6.443726000	0.641641000	0.192763000
H	-5.228166000	1.666983000	-0.596589000
H	-6.599991000	1.041406000	-1.526313000
C	-6.249310000	-2.109820000	-1.581296000
H	-6.989393000	-1.760630000	-2.317805000
H	-5.817671000	-3.044940000	-1.964218000
H	-6.790463000	-2.350760000	-0.654457000
C	1.295244000	3.501929000	-3.280328000
H	1.516763000	4.556221000	-3.510639000
H	2.252601000	2.966201000	-3.240481000
H	0.716838000	3.099118000	-4.121776000
C	2.597142000	3.623886000	-0.413988000
H	2.819289000	4.689157000	-0.232183000
H	2.934984000	3.055262000	0.455536000
H	3.196747000	3.303990000	-1.275241000
C	-1.882688000	3.340484000	-2.964962000
H	-2.179945000	4.370913000	-3.217761000
H	-1.477244000	2.886944000	-3.879223000
H	-2.797925000	2.796353000	-2.697218000
C	-2.585215000	3.485366000	0.114767000
H	-2.661334000	3.073673000	1.125817000
H	-2.878097000	4.547388000	0.157986000
H	-3.322786000	2.968280000	-0.511600000
C	-0.833238000	2.405963000	3.201920000
H	-0.639070000	2.576783000	4.273161000
H	-1.919103000	2.482690000	3.052319000
H	-0.530472000	1.379068000	2.955736000
C	-0.543487000	5.412191000	2.531334000
H	-0.493104000	5.644748000	3.606192000
H	0.027504000	6.184902000	1.995433000
H	-1.594729000	5.504937000	2.222543000
C	1.929526000	3.631890000	2.856853000
H	2.404109000	2.655055000	2.691767000
H	2.575881000	4.407931000	2.425462000
H	1.890761000	3.800203000	3.944537000

Complex 8a

Ti	0.231234000	1.468540000	0.880930000
H	1.510305000	0.583139000	-0.248530000
H	-1.371519000	1.080293000	-0.092590000
Ti	-1.576930000	-0.717725000	0.353271000
Ti	1.155782000	-1.211418000	0.183336000
Si	0.799836000	3.960043000	-1.970905000
Si	-4.831970000	-0.775714000	-1.704200000
Si	4.727893000	-1.406212000	-1.223989000
N	-0.131754000	-0.317092000	1.459856000
N	-0.485819000	-1.522849000	-0.910200000
C	0.152283000	-1.876358000	-2.163528000
C	-0.272508000	-3.274140000	-2.659746000
H	0.324809000	-3.581305000	-3.530232000
H	-1.329437000	-3.245855000	-2.956728000

H	-0.159195000	-4.023238000	-1.868357000
C	-0.083853000	-0.803589000	-3.247070000
H	-1.152737000	-0.759056000	-3.495343000
H	0.477945000	-1.043859000	-4.161592000
H	0.230902000	0.179871000	-2.880723000
C	0.589090000	3.586975000	-0.128195000
C	-0.634566000	3.700245000	0.639185000
C	-0.333283000	3.505680000	2.020605000
C	1.081249000	3.287320000	2.143144000
C	1.654510000	3.356945000	0.832423000
C	-1.990775000	4.082307000	0.091277000
H	-2.312388000	3.418434000	-0.718039000
H	-1.966789000	5.110395000	-0.303040000
H	-2.758310000	4.053559000	0.873438000
C	-1.288833000	3.593737000	3.186975000
H	-2.330467000	3.450461000	2.875641000
H	-1.223075000	4.582695000	3.668893000
H	-1.064782000	2.842817000	3.956994000
C	1.816665000	3.142182000	3.455658000
H	1.254816000	2.527762000	4.172960000
H	1.972883000	4.127344000	3.924415000
H	2.803343000	2.682377000	3.324594000
C	3.135334000	3.371034000	0.530941000
H	3.726130000	3.127305000	1.422034000
H	3.449067000	4.373426000	0.198156000
H	3.405014000	2.660427000	-0.257903000
C	2.266854000	3.021010000	-2.737483000
H	3.239711000	3.439915000	-2.445779000
H	2.202608000	3.077852000	-3.835192000
H	2.254238000	1.959433000	-2.453647000
C	1.118415000	5.829382000	-2.174278000
H	0.280200000	6.425209000	-1.783674000
H	1.251506000	6.096466000	-3.233952000
H	2.024600000	6.144120000	-1.635732000
C	-0.743206000	3.507079000	-2.987019000
H	-1.095690000	2.491743000	-2.759183000
H	-0.494256000	3.542878000	-4.059034000
H	-1.579110000	4.200605000	-2.822897000
C	-3.921914000	-1.062539000	-0.067637000
C	-3.820474000	-0.066946000	0.988895000
C	-3.237559000	-0.670019000	2.140422000
C	-2.946193000	-2.033803000	1.818877000
C	-3.383041000	-2.285315000	0.475493000
C	-4.398126000	1.328112000	0.953188000
H	-3.856463000	2.004105000	1.624964000
H	-5.451759000	1.316922000	1.275755000
H	-4.360984000	1.763851000	-0.050546000
C	-2.981483000	-0.036593000	3.484482000
H	-1.942831000	-0.196243000	3.806848000
H	-3.642824000	-0.467233000	4.253281000
H	-3.164019000	1.044080000	3.463057000
C	-2.400305000	-3.040990000	2.800492000
H	-1.968708000	-3.913749000	2.296996000
H	-3.202495000	-3.407482000	3.461939000
H	-1.624569000	-2.596921000	3.437548000
C	-3.332094000	-3.642417000	-0.187158000
H	-3.099197000	-3.572797000	-1.253215000
H	-4.298844000	-4.161804000	-0.086000000
H	-2.569463000	-4.280391000	0.277214000
C	-4.780608000	-2.274721000	-2.874873000
H	-3.763027000	-2.514329000	-3.214575000
H	-5.373727000	-2.033169000	-3.770825000
H	-5.213398000	-3.181072000	-2.430156000
C	-6.666388000	-0.436843000	-1.317353000
H	-7.122262000	-1.283527000	-0.783359000
H	-7.237115000	-0.281123000	-2.245784000
H	-6.800203000	0.458005000	-0.693320000

C	-4.137638000	0.699891000	-2.687832000
H	-4.312458000	1.667192000	-2.197085000
H	-4.620631000	0.744896000	-3.676685000
H	-3.054967000	0.605101000	-2.848862000
C	3.442292000	-1.829308000	0.101154000
C	3.236606000	-1.218693000	1.404830000
C	2.333360000	-2.021655000	2.156955000
C	1.962428000	-3.149216000	1.349352000
C	2.656959000	-3.050284000	0.105765000
C	3.921309000	0.007214000	1.954160000
H	4.043635000	0.784185000	1.195362000
H	4.922438000	-0.242938000	2.343268000
H	3.347595000	0.431525000	2.787817000
C	1.878025000	-1.750828000	3.568118000
H	1.631199000	-0.691420000	3.713668000
H	2.660671000	-2.023801000	4.294099000
H	0.978782000	-2.327731000	3.814862000
C	1.100512000	-4.311678000	1.778581000
H	0.439059000	-4.038525000	2.608011000
H	1.725842000	-5.153555000	2.117792000
H	0.472082000	-4.681974000	0.957264000
C	2.694753000	-4.147259000	-0.933084000
H	1.778700000	-4.750919000	-0.921204000
H	3.534501000	-4.832135000	-0.733078000
H	2.827210000	-3.759827000	-1.951312000
C	6.015737000	-2.810417000	-1.288569000
H	6.493054000	-2.955010000	-0.308084000
H	6.809514000	-2.571783000	-2.013195000
H	5.576314000	-3.772424000	-1.587037000
C	3.968722000	-1.208938000	-2.959826000
H	3.472258000	-2.119774000	-3.324199000
H	4.760755000	-0.960119000	-3.683574000
H	3.232007000	-0.393331000	-2.981556000
C	5.690348000	0.194946000	-0.873074000
H	5.050534000	1.087411000	-0.890028000
H	6.448256000	0.321545000	-1.662000000
H	6.219576000	0.172482000	0.089222000
H	1.270525000	-1.911272000	-1.999820000

A'

C	-0.325607000	0.592524000	1.099585000
H	-1.483439000	-0.162063000	-0.934885000
Ti	-0.753405000	-1.367576000	0.326384000
Si	-1.955419000	3.595142000	1.731671000
Si	4.465822000	-0.923553000	-1.679230000
Si	-4.381581000	-2.002081000	-0.848718000
Ti	-0.248968000	1.239206000	-0.781277000
C	-0.366964000	-0.386882000	2.062226000
C	-0.535171000	-0.329246000	3.560511000
H	0.050847000	0.485336000	4.014817000
H	-0.239778000	-1.270794000	4.041370000
H	-1.591736000	-0.148380000	3.817352000
C	-1.255127000	3.222585000	0.010640000
C	-2.029644000	2.811757000	-1.136400000
C	-1.217875000	2.923707000	-2.308796000
C	0.088569000	3.349301000	-1.905424000
C	0.065161000	3.546172000	-0.482656000
C	3.854565000	-0.517663000	0.069753000
C	3.797633000	0.774120000	0.727964000
C	3.382150000	0.588659000	2.084373000
C	3.182095000	-0.813521000	2.302717000
C	3.493092000	-1.492073000	1.078008000
C	-2.701403000	-2.556033000	-0.167912000
C	-2.377197000	-2.842519000	1.218319000
C	-1.142651000	-3.550300000	1.258167000
C	-0.693996000	-3.740609000	-0.096666000
C	-1.640690000	-3.136086000	-0.971124000

H	1.010405000	-1.859693000	0.576803000
Ti	1.613454000	-0.148838000	0.651464000
H	0.621026000	-0.637088000	-0.910605000
H	1.559627000	1.252663000	-0.534828000
N	0.217513000	0.089617000	-3.832905000
N	0.004963000	0.476486000	-2.794511000
C	-5.411874000	-3.583988000	-1.113579000
H	-6.409015000	-3.344498000	-1.513923000
H	-4.923715000	-4.267769000	-1.823508000
H	-5.553912000	-4.133549000	-0.171336000
C	-5.350966000	-0.889824000	0.352704000
H	-4.764484000	-0.034044000	0.712783000
H	-6.235251000	-0.488834000	-0.166620000
H	-5.712363000	-1.442815000	1.230583000
C	-4.246128000	-1.098180000	-2.516622000
H	-5.189264000	-0.570478000	-2.726693000
H	-3.436291000	-0.356765000	-2.505372000
H	-4.064741000	-1.789591000	-3.350830000
C	-3.232460000	-2.524000000	2.423255000
H	-3.616931000	-1.497799000	2.400529000
H	-4.100482000	-3.200994000	2.475226000
H	-2.665697000	-2.646525000	3.353803000
C	-0.454305000	-4.098058000	2.482734000
H	-0.744353000	-3.554007000	3.389182000
H	-0.711721000	-5.158871000	2.635599000
H	0.637503000	-4.034167000	2.391546000
C	0.503379000	-4.556212000	-0.519235000
H	1.226700000	-4.658777000	0.296878000
H	0.188338000	-5.570438000	-0.813327000
H	1.024871000	-4.110363000	-1.374922000
C	-1.570672000	-3.185286000	-2.480229000
H	-2.296044000	-3.909337000	-2.886227000
H	-1.782881000	-2.210892000	-2.933172000
H	-0.574650000	-3.499240000	-2.816090000
C	3.608004000	-2.992373000	0.956182000
H	3.371115000	-3.345536000	-0.051723000
H	4.637644000	-3.309278000	1.190143000
H	2.940173000	-3.504188000	1.659558000
C	2.868641000	-1.474065000	3.622422000
H	2.223699000	-2.352238000	3.494771000
H	3.794603000	-1.810547000	4.117557000
H	2.360699000	-0.785509000	4.307888000
C	3.249125000	1.660610000	3.139798000
H	2.469251000	1.412839000	3.871103000
H	4.194273000	1.776429000	3.694760000
H	3.000257000	2.636599000	2.707024000
C	4.253772000	2.094203000	0.153400000
H	5.352417000	2.110567000	0.072816000
H	3.839947000	2.277346000	-0.842361000
H	3.961852000	2.928902000	0.800528000
C	4.530726000	0.598649000	-2.815407000
H	3.549865000	1.087863000	-2.895613000
H	5.266145000	1.349109000	-2.495852000
H	4.817675000	0.267142000	-3.825529000
C	6.226486000	-1.640732000	-1.545091000
H	6.247306000	-2.552695000	-0.930608000
H	6.623034000	-1.901014000	-2.538415000
H	6.919336000	-0.919059000	-1.087739000
C	3.356821000	-2.196173000	-2.560717000
H	3.491001000	-3.221123000	-2.187790000
H	2.295048000	-1.932073000	-2.459277000
H	3.599635000	-2.208379000	-3.634663000
C	-3.283663000	2.352851000	2.289392000
H	-3.485923000	2.494294000	3.362493000
H	-4.236231000	2.486653000	1.758654000
H	-2.947542000	1.317733000	2.143428000
C	-2.771745000	5.316675000	1.630712000

H	-3.206516000	5.605956000	2.599832000
H	-2.042885000	6.090977000	1.348749000
H	-3.580357000	5.339404000	0.885084000
C	-0.627405000	3.667360000	3.089118000
H	-0.001759000	2.765340000	3.086286000
H	0.027641000	4.543999000	2.992882000
H	-1.121773000	3.732729000	4.070900000
C	1.190999000	4.159068000	0.314191000
H	0.961449000	5.207072000	0.568278000
H	1.370360000	3.617089000	1.247976000
H	2.123347000	4.159140000	-0.261056000
C	1.240423000	3.652360000	-2.832144000
H	1.199647000	4.696185000	-3.184011000
H	2.206758000	3.508900000	-2.333941000
H	1.228410000	3.007584000	-3.720938000
C	-1.701191000	2.751546000	-3.728106000
H	-2.254303000	3.648511000	-4.048801000
H	-0.869045000	2.613967000	-4.429056000
H	-2.376878000	1.892919000	-3.836604000
C	-3.503744000	2.481598000	-1.148061000
H	-3.766723000	1.749539000	-0.378523000
H	-4.104870000	3.387580000	-0.968087000
H	-3.811927000	2.072253000	-2.117033000

TS1'

C	-0.398602000	0.489858000	1.025690000
H	-1.556130000	0.217885000	0.238620000
Ti	-0.744649000	-1.481845000	0.227400000
Si	-1.861257000	3.612331000	1.835233000
Si	4.445167000	-0.805569000	-1.717651000
Si	-4.422390000	-1.970074000	-0.692923000
Ti	-0.360223000	1.290051000	-0.823035000
C	-0.078945000	-0.464215000	1.992784000
C	-0.368157000	-0.502032000	3.479774000
H	0.080298000	0.357802000	4.004553000
H	0.025136000	-1.415044000	3.945237000
H	-1.450690000	-0.467934000	3.682103000
C	-1.260797000	3.266687000	0.070116000
C	-2.105409000	2.897163000	-1.049063000
C	-1.349349000	3.004664000	-2.254392000
C	-0.014066000	3.404332000	-1.904516000
C	0.037006000	3.577791000	-0.480219000
C	3.859185000	-0.497537000	0.060363000
C	3.809992000	0.751565000	0.792252000
C	3.423538000	0.480265000	2.144566000
C	3.240764000	-0.933225000	2.283899000
C	3.513174000	-1.532743000	1.012684000
C	-2.723988000	-2.630830000	-0.174723000
C	-2.290858000	-2.989800000	1.164342000
C	-1.056801000	-3.699887000	1.075286000
C	-0.707260000	-3.803752000	-0.315043000
C	-1.725168000	-3.158423000	-1.084706000
H	1.027759000	-1.639770000	-0.220541000
Ti	1.626919000	-0.165524000	0.705140000
H	-0.781266000	-0.675402000	-1.322889000
H	1.454014000	1.113438000	-0.646198000
N	0.363473000	0.299818000	-3.854204000
N	0.063269000	0.623195000	-2.812773000
C	6.195850000	-1.555421000	-1.633715000
H	6.205207000	-2.502545000	-1.074612000
H	6.584358000	-1.762265000	-2.642722000
H	6.901315000	-0.872550000	-1.137668000
C	4.537604000	0.783664000	-2.756126000
H	4.837009000	0.512312000	-3.780485000
H	3.561335000	1.283799000	-2.821149000
H	5.273323000	1.507274000	-2.380262000
C	3.314370000	-2.004819000	-2.669379000

H	2.255874000	-1.752787000	-2.520339000
H	3.532227000	-1.934079000	-3.746387000
H	3.458886000	-3.054749000	-2.378372000
C	3.586462000	-3.022772000	0.783634000
H	3.330133000	-3.292681000	-0.245003000
H	4.606803000	-3.388511000	0.985295000
H	2.908167000	-3.564916000	1.453952000
C	2.966395000	-1.675053000	3.568300000
H	2.314621000	-2.542929000	3.407227000
H	3.907260000	-2.044976000	4.007829000
H	2.486572000	-1.030412000	4.314037000
C	3.286337000	1.490607000	3.258634000
H	2.522180000	1.188036000	3.986297000
H	4.236611000	1.597337000	3.806114000
H	3.012514000	2.484127000	2.882585000
C	4.234243000	2.109252000	0.283320000
H	5.329874000	2.148760000	0.174492000
H	3.791801000	2.342716000	-0.689742000
H	3.949025000	2.902876000	0.983599000
C	-0.297465000	-4.318237000	2.223115000
H	0.773442000	-4.397338000	2.000074000
H	-0.403043000	-3.732995000	3.144734000
H	-0.665489000	-5.336082000	2.432118000
C	0.459721000	-4.576016000	-0.881335000
H	1.249513000	-4.717805000	-0.135348000
H	0.133009000	-5.574930000	-1.212904000
H	0.904587000	-4.068260000	-1.745626000
C	-1.779916000	-3.171721000	-2.595171000
H	-2.419822000	-3.994119000	-2.956548000
H	-2.171251000	-2.234090000	-3.000363000
H	-0.780844000	-3.323658000	-3.022050000
C	-3.041984000	-2.730593000	2.450645000
H	-3.395977000	-1.695575000	2.527781000
H	-3.925296000	-3.385099000	2.522664000
H	-2.411832000	-2.934100000	3.324416000
C	-5.263665000	-0.929760000	0.659981000
H	-6.177680000	-0.478144000	0.243818000
H	-5.564716000	-1.530950000	1.528736000
H	-4.626968000	-0.110251000	1.020910000
C	-5.536677000	-3.477705000	-1.035747000
H	-6.542278000	-3.162383000	-1.353875000
H	-5.119280000	-4.111539000	-1.831843000
H	-5.651624000	-4.105788000	-0.140071000
C	-4.346451000	-0.912164000	-2.273048000
H	-3.468835000	-0.251022000	-2.267787000
H	-4.308258000	-1.524632000	-3.184402000
H	-5.247094000	-0.282583000	-2.339568000
C	-3.179426000	2.384595000	2.445625000
H	-3.344157000	2.541020000	3.523104000
H	-4.149045000	2.515467000	1.946468000
H	-2.854536000	1.344926000	2.306369000
C	-2.647819000	5.350103000	1.813680000
H	-3.024367000	5.626455000	2.810493000
H	-1.920188000	6.116632000	1.508443000
H	-3.494557000	5.403564000	1.113356000
C	-0.464827000	3.624125000	3.124028000
H	-0.909958000	3.695520000	4.128697000
H	0.125353000	2.699235000	3.085195000
H	0.217160000	4.477078000	3.006717000
C	1.215944000	4.148644000	0.269629000
H	1.020755000	5.192707000	0.564830000
H	1.438497000	3.579048000	1.177765000
H	2.115330000	4.148563000	-0.355625000
C	1.096396000	3.716369000	-2.877981000
H	1.076189000	4.779963000	-3.165922000
H	2.083358000	3.508982000	-2.446300000
H	1.008664000	3.127512000	-3.799955000

C	-1.890614000	2.842540000	-3.653876000
H	-2.390653000	3.768801000	-3.978799000
H	-1.094283000	2.631027000	-4.377660000
H	-2.625166000	2.029512000	-3.720111000
C	-3.589596000	2.612956000	-0.991865000
H	-3.844832000	1.878854000	-0.220776000
H	-4.148528000	3.536602000	-0.770207000
H	-3.957852000	2.230519000	-1.950673000

B'

C	-0.323403000	0.223583000	1.275840000
H	-0.776482000	0.861653000	2.047785000
Ti	-0.812817000	-1.079482000	-0.482636000
Si	-3.101584000	3.315032000	0.882551000
Si	5.087774000	-0.286924000	-0.949047000
Si	-4.609077000	-2.210539000	0.421553000
Ti	0.134708000	1.472077000	-0.378542000
C	-0.210294000	-1.179786000	1.507772000
C	-0.643132000	-1.878892000	2.780725000
H	-0.111712000	-1.479254000	3.658738000
H	-0.469258000	-2.960464000	2.750536000
H	-1.716230000	-1.722492000	2.962137000
C	-1.356671000	3.262114000	0.144537000
C	-0.961072000	3.375221000	-1.248724000
C	0.437155000	3.668374000	-1.308371000
C	0.936274000	3.712103000	0.033529000
C	-0.156808000	3.466512000	0.922574000
C	3.937742000	-0.831771000	0.460760000
C	3.683480000	-0.103448000	1.689135000
C	2.980098000	-0.948441000	2.594830000
C	2.787514000	-2.220108000	1.956779000
C	3.377163000	-2.152563000	0.651722000
C	-2.987793000	-2.186448000	-0.570843000
C	-1.947606000	-3.186222000	-0.432781000
C	-1.109824000	-3.146587000	-1.594620000
C	-1.605437000	-2.117472000	-2.460823000
C	-2.750453000	-1.528192000	-1.836880000
H	0.928793000	-1.629984000	-0.785546000
Ti	1.615807000	-0.602766000	0.598153000
H	-1.264210000	0.565026000	-1.143052000
H	1.861339000	1.154004000	0.128618000
N	1.444810000	0.538248000	-3.119577000
N	0.972359000	0.819269000	-2.119043000
C	-5.831836000	-0.838364000	-0.067293000
H	-6.744530000	-0.968239000	0.535436000
H	-5.450029000	0.171046000	0.135988000
H	-6.129188000	-0.885520000	-1.123319000
C	-5.453029000	-3.871912000	0.020128000
H	-4.846565000	-4.731505000	0.339004000
H	-6.426763000	-3.946536000	0.528267000
H	-5.631008000	-3.976071000	-1.060254000
C	-4.425350000	-2.095802000	2.312176000
H	-3.970167000	-1.147301000	2.627231000
H	-5.430106000	-2.142588000	2.761448000
H	-3.838077000	-2.914551000	2.748919000
C	-3.475546000	1.891083000	2.084840000
H	-4.530181000	1.932801000	2.399031000
H	-3.299131000	0.921309000	1.600884000
H	-2.862090000	1.923942000	2.996498000
C	-4.478178000	3.319561000	-0.430091000
H	-5.443051000	3.455024000	0.083288000
H	-4.371257000	4.144794000	-1.147515000
H	-4.541206000	2.383451000	-1.000507000
C	-3.271936000	4.963512000	1.825190000
H	-4.287443000	5.067895000	2.237516000
H	-2.565710000	5.044094000	2.663095000
H	-3.093729000	5.820403000	1.158767000

C	-0.055024000	3.541198000	2.428360000
H	-0.078348000	4.587698000	2.772818000
H	-0.882881000	3.015916000	2.919679000
H	0.880655000	3.095386000	2.790885000
C	2.323567000	4.138566000	0.442062000
H	2.384478000	5.238679000	0.484930000
H	2.586539000	3.755189000	1.434117000
H	3.086612000	3.794897000	-0.266311000
C	1.236198000	3.986579000	-2.549086000
H	1.201893000	5.066892000	-2.763768000
H	2.291747000	3.708490000	-2.434463000
H	0.850106000	3.464464000	-3.433319000
C	-1.855712000	3.302922000	-2.465381000
H	-2.672772000	2.588981000	-2.328297000
H	-2.299025000	4.287047000	-2.689123000
H	-1.288186000	2.993919000	-3.353070000
C	2.604572000	-0.575287000	4.009490000
H	3.505819000	-0.460164000	4.632069000
H	2.054174000	0.375058000	4.051079000
H	1.978946000	-1.342886000	4.479022000
C	2.264644000	-3.482134000	2.598550000
H	3.099988000	-4.163713000	2.826292000
H	1.743584000	-3.274825000	3.539231000
H	1.569054000	-4.022884000	1.943929000
C	3.495978000	-3.341622000	-0.276699000
H	3.254742000	-3.089858000	-1.314123000
H	4.520121000	-3.748714000	-0.258062000
H	2.819690000	-4.146482000	0.035179000
C	4.187301000	1.272764000	2.048638000
H	5.206133000	1.210758000	2.466715000
H	4.219020000	1.936809000	1.181164000
H	3.550685000	1.742275000	2.809681000
C	4.930797000	1.557392000	-1.388788000
H	3.878674000	1.852869000	-1.496086000
H	5.400248000	2.218199000	-0.647186000
H	5.430932000	1.740817000	-2.352282000
C	6.873467000	-0.619168000	-0.373611000
H	7.031826000	-1.685045000	-0.153270000
H	7.598730000	-0.326266000	-1.148121000
H	7.114096000	-0.054249000	0.538979000
C	4.793122000	-1.249511000	-2.562324000
H	5.411755000	-0.798514000	-3.353859000
H	5.078015000	-2.307526000	-2.489590000
H	3.747572000	-1.194666000	-2.896805000
C	-1.859001000	-4.265522000	0.619542000
H	-2.329670000	-5.194508000	0.257819000
H	-0.816287000	-4.505309000	0.865448000
H	-2.362564000	-3.977122000	1.547637000
C	-0.003306000	-4.119325000	-1.921144000
H	-0.411766000	-5.004654000	-2.436139000
H	0.750619000	-3.670001000	-2.578672000
H	0.508106000	-4.469156000	-1.016769000
C	-1.033548000	-1.763721000	-3.812108000
H	-1.427663000	-2.437583000	-4.590093000
H	-1.286623000	-0.737817000	-4.105369000
H	0.060993000	-1.849591000	-3.826955000
C	-3.603522000	-0.464275000	-2.486173000
H	-4.440217000	-0.920396000	-3.040025000
H	-4.025175000	0.225341000	-1.749471000
H	-3.019029000	0.126995000	-3.200946000

TS7''

Ti	-0.035998000	1.425788000	-0.870592000
Ti	-1.449561000	-0.551538000	0.355038000
Ti	1.281387000	-1.005466000	-0.603356000
Si	0.725316000	3.865489000	1.983215000
Si	-5.055755000	-1.326735000	-0.520582000

Si	4.220178000	-1.810360000	1.603999000
N	0.311822000	0.095275000	0.597662000
N	-1.824813000	0.910255000	-0.735974000
C	-0.705024000	-1.764457000	-1.279421000
H	-1.327300000	-2.608119000	-1.596025000
C	-0.181537000	-0.795105000	-2.085979000
C	-0.602271000	0.155319000	-3.071156000
H	-1.437161000	0.806035000	-2.075638000
H	-1.454114000	-0.070338000	-3.731360000
H	0.181505000	0.733760000	-3.569930000
C	0.445294000	3.508464000	0.137120000
C	1.514608000	3.303978000	-0.815126000
C	0.964509000	3.286857000	-2.130526000
C	-0.448767000	3.535315000	-2.021800000
C	-0.769604000	3.679396000	-0.643289000
C	-3.676138000	-1.377701000	0.777041000
C	-2.791095000	-2.503069000	0.993461000
C	-1.943266000	-2.219846000	2.107745000
C	-2.271486000	-0.914028000	2.590142000
C	-3.342313000	-0.397973000	1.783277000
C	3.338503000	-1.967895000	-0.071215000
C	2.454568000	-3.068564000	-0.426825000
C	2.142729000	-2.982063000	-1.814270000
C	2.788083000	-1.820957000	-2.343912000
C	3.541587000	-1.209261000	-1.286096000
H	1.679112000	0.617627000	-1.284291000
C	-0.951736000	-3.163289000	2.740379000
H	-1.403686000	-3.685970000	3.599611000
H	-0.615930000	-3.930544000	2.032641000
H	-0.064452000	-2.634454000	3.111797000
C	-2.841475000	-3.836780000	0.286515000
H	-3.437764000	-4.560557000	0.864857000
H	-3.298308000	-3.757016000	-0.706895000
H	-1.838657000	-4.267682000	0.159326000
C	-1.657554000	-0.262907000	3.806984000
H	-2.182446000	-0.576699000	4.724038000
H	-0.601381000	-0.539111000	3.919574000
H	-1.707909000	0.831500000	3.760071000
C	-4.025052000	0.930212000	2.020398000
H	-4.141743000	1.501470000	1.093642000
H	-5.024250000	0.783768000	2.459730000
H	-3.451788000	1.546349000	2.724477000
C	-6.316576000	-2.694296000	-0.102292000
H	-7.144906000	-2.696628000	-0.827435000
H	-5.863670000	-3.696030000	-0.114152000
H	-6.749416000	-2.540740000	0.897340000
C	-4.409511000	-1.603447000	-2.290076000
H	-3.927943000	-2.579873000	-2.439719000
H	-5.243601000	-1.535549000	-3.006304000
H	-3.676249000	-0.826762000	-2.547222000
C	-5.992495000	0.325912000	-0.558866000
H	-6.463079000	0.579521000	0.400616000
H	-5.336691000	1.158014000	-0.850286000
H	-6.794012000	0.256045000	-1.310993000
C	-0.891158000	4.062901000	2.964075000
H	-0.633975000	4.276978000	4.013332000
H	-1.513184000	4.892590000	2.602341000
H	-1.503626000	3.151008000	2.956746000
C	1.740563000	2.511161000	2.846583000
H	2.809675000	2.553370000	2.594826000
H	1.659537000	2.623077000	3.939063000
H	1.365287000	1.516470000	2.569882000
C	1.653679000	5.525458000	2.109010000
H	1.824008000	5.794287000	3.162885000
H	2.635072000	5.490519000	1.614978000
H	1.078199000	6.340320000	1.645662000
C	-2.150288000	4.000413000	-0.129184000

H	-2.368571000	3.477884000	0.806155000
H	-2.260520000	5.082926000	0.047266000
H	-2.913784000	3.698944000	-0.856015000
C	-1.424234000	3.644148000	-3.168412000
H	-2.392588000	3.192949000	-2.914840000
H	-1.606881000	4.698403000	-3.430329000
H	-1.048312000	3.142756000	-4.069593000
C	1.747484000	3.147559000	-3.413144000
H	1.111539000	2.815999000	-4.244378000
H	2.190213000	4.112149000	-3.709171000
H	2.567839000	2.425138000	-3.310246000
C	2.986318000	3.212273000	-0.500636000
H	3.412524000	4.217323000	-0.350131000
H	3.176134000	2.631292000	0.409042000
H	3.539551000	2.741231000	-1.320660000
C	2.772606000	-1.382162000	-3.787456000
H	2.806672000	-0.288777000	-3.876747000
H	3.639735000	-1.787231000	-4.334243000
H	1.866381000	-1.726793000	-4.300831000
C	1.318981000	-3.967389000	-2.601845000
H	0.762289000	-3.475777000	-3.409871000
H	1.966114000	-4.732060000	-3.061057000
H	0.592750000	-4.487407000	-1.964934000
C	2.034179000	-4.209851000	0.469639000
H	2.737632000	-5.053280000	0.378066000
H	2.008016000	-3.916750000	1.524757000
H	1.037909000	-4.585527000	0.202357000
C	4.508504000	-0.070242000	-1.502667000
H	4.555689000	0.606660000	-0.645986000
H	5.524716000	-0.459156000	-1.680209000
H	4.224906000	0.519848000	-2.382675000
C	5.326233000	-0.269783000	1.733514000
H	5.814004000	-0.280330000	2.720806000
H	6.120777000	-0.243486000	0.975715000
H	4.754341000	0.666259000	1.664758000
C	3.005245000	-1.721211000	3.066512000
H	2.255773000	-0.932165000	2.913191000
H	2.470599000	-2.664983000	3.242659000
H	3.558387000	-1.485307000	3.989063000
C	5.339712000	-3.335426000	1.819996000
H	5.882988000	-3.286229000	2.776039000
H	4.767455000	-4.273816000	1.812526000
H	6.086150000	-3.396771000	1.014521000

G''

Ti	-0.079829000	1.463392000	-0.821917000
Ti	-1.355122000	-0.672612000	0.437406000
Ti	1.401235000	-0.882277000	-0.581301000
Si	0.300710000	3.922273000	2.032992000
Si	-4.898221000	-1.628717000	-0.683844000
Si	4.298097000	-1.698777000	1.630654000
N	0.342765000	0.104228000	0.630212000
N	-1.895118000	0.927088000	-0.438526000
C	-0.613397000	-1.641125000	-1.285249000
H	-1.003263000	-2.565238000	-1.724630000
C	-0.075054000	-0.617783000	-2.054695000
C	-0.295189000	0.352700000	-3.012730000
H	-2.791118000	1.376311000	-0.643299000
H	-1.223840000	0.419358000	-3.591525000
H	0.567910000	0.879565000	-3.424954000
C	0.164925000	3.575192000	0.170445000
C	1.297405000	3.408166000	-0.711239000
C	0.834474000	3.359236000	-2.060371000
C	-0.591973000	3.510900000	-2.044155000
C	-1.003051000	3.660417000	-0.685168000
C	-3.576141000	-1.641131000	0.674728000
C	-2.619853000	-2.707655000	0.864636000

C	-1.832786000	-2.423004000	2.022285000
C	-2.282924000	-1.175826000	2.567098000
C	-3.359486000	-0.699937000	1.749655000
C	3.469280000	-1.814539000	-0.072089000
C	2.624875000	-2.921181000	-0.497623000
C	2.325201000	-2.767965000	-1.881654000
C	2.950031000	-1.565849000	-2.342978000
C	3.667187000	-0.986636000	-1.243456000
H	1.701757000	0.787547000	-1.199790000
C	-6.014890000	-0.087633000	-0.631595000
H	-6.796106000	-0.202024000	-1.399362000
H	-6.520885000	0.045242000	0.334251000
H	-5.472109000	0.840967000	-0.860506000
C	-6.033738000	-3.138099000	-0.432432000
H	-6.824720000	-3.161334000	-1.197731000
H	-5.484204000	-4.087779000	-0.495850000
H	-6.523414000	-3.105614000	0.552089000
C	-4.150562000	-1.688184000	-2.432032000
H	-4.947510000	-1.582953000	-3.185192000
H	-3.432288000	-0.868460000	-2.572126000
H	-3.618750000	-2.625881000	-2.644896000
C	-2.531528000	-3.989140000	0.071383000
H	-3.107534000	-4.790750000	0.560974000
H	-2.928510000	-3.869306000	-0.943395000
H	-1.494026000	-4.338018000	-0.018233000
C	-0.803944000	-3.331377000	2.649516000
H	-1.262857000	-3.943358000	3.443579000
H	-0.370654000	-4.021053000	1.915780000
H	0.017431000	-2.766255000	3.107975000
C	-1.765964000	-0.543230000	3.838298000
H	-2.335795000	-0.898722000	4.712325000
H	-0.710864000	-0.791974000	4.008597000
H	-1.846163000	0.550624000	3.817186000
C	-4.167354000	0.538875000	2.058346000
H	-4.396106000	1.125433000	1.162057000
H	-5.125544000	0.271389000	2.531688000
H	-3.632688000	1.193576000	2.757356000
C	-2.416755000	3.971268000	-0.261007000
H	-2.714164000	3.406899000	0.629055000
H	-2.527195000	5.043475000	-0.033849000
H	-3.128669000	3.740444000	-1.064911000
C	-1.490943000	3.577878000	-3.254503000
H	-2.464170000	3.106989000	-3.064352000
H	-1.679459000	4.623277000	-3.547302000
H	-1.043283000	3.068305000	-4.116513000
C	1.711261000	3.276580000	-3.285202000
H	1.136059000	3.000618000	-4.177751000
H	2.184594000	4.250204000	-3.489367000
H	2.513711000	2.537514000	-3.160292000
C	2.750259000	3.382251000	-0.302089000
H	3.090863000	4.393317000	-0.026624000
H	2.921695000	2.724999000	0.557504000
H	3.384806000	3.030768000	-1.123024000
C	-1.376409000	3.849117000	2.924782000
H	-1.206854000	3.998084000	4.002595000
H	-2.075427000	4.628495000	2.592558000
H	-1.866619000	2.874080000	2.798935000
C	0.979475000	5.691959000	2.235523000
H	1.078563000	5.952277000	3.300531000
H	1.970946000	5.805915000	1.773779000
H	0.311713000	6.432706000	1.771502000
C	1.459137000	2.704012000	2.919845000
H	1.266024000	1.674688000	2.587246000
H	2.521859000	2.927221000	2.750498000
H	1.286063000	2.754104000	4.006219000
C	5.360624000	-0.136921000	1.850016000
H	5.829098000	-0.177899000	2.845874000

H	6.168554000	-0.056808000	1.110367000
H	4.765815000	0.786677000	1.809549000
C	5.448318000	-3.202362000	1.836644000
H	5.957546000	-3.172589000	2.812074000
H	4.900849000	-4.153605000	1.777613000
H	6.222739000	-3.217889000	1.055741000
C	3.036055000	-1.685284000	3.056957000
H	3.554140000	-1.481432000	4.007169000
H	2.280003000	-0.900720000	2.910300000
H	2.508564000	-2.642231000	3.174351000
C	2.232426000	-4.121377000	0.332716000
H	2.960608000	-4.938359000	0.201990000
H	2.191699000	-3.887455000	1.402508000
H	1.249088000	-4.511373000	0.038619000
C	1.542851000	-3.729088000	-2.738870000
H	2.222552000	-4.403484000	-3.284599000
H	0.871079000	-4.353444000	-2.137083000
H	0.932249000	-3.201263000	-3.483165000
C	2.957788000	-1.073879000	-3.768611000
H	3.823625000	-1.476440000	-4.320001000
H	2.049878000	-1.380211000	-4.302374000
H	3.015992000	0.020907000	-3.819189000
C	4.588374000	0.202996000	-1.377224000
H	4.572744000	0.846179000	-0.492980000
H	5.628369000	-0.128361000	-1.532298000
H	4.307622000	0.816888000	-2.241843000

TS7'

Ti	0.496576000	1.344759000	0.716283000
Ti	1.237276000	-0.962153000	-0.313993000
Ti	-1.554891000	-0.913722000	0.516874000
Si	0.195591000	4.093575000	-1.861763000
Si	4.912284000	-1.582248000	0.126382000
Si	-4.646570000	-0.599213000	-1.548582000
N	-0.474594000	0.018445000	-0.693721000
N	2.074952000	0.555124000	0.235489000
C	0.066974000	-1.734295000	1.478441000
H	0.275932000	-2.643515000	2.060231000
C	0.345834000	-0.463760000	1.981411000
C	0.927751000	-0.307315000	3.386201000
H	1.152267000	-1.282612000	3.847973000
H	0.201257000	0.215562000	4.025717000
H	1.848000000	0.289630000	3.385165000
C	0.391114000	3.584679000	-0.041246000
C	-0.703327000	3.446872000	0.898329000
C	-0.166060000	3.185740000	2.197051000
C	1.267165000	3.199143000	2.086504000
C	1.613079000	3.450291000	0.725552000
C	3.318319000	-1.995537000	-0.813708000
C	2.421890000	-3.078157000	-0.476146000
C	1.390449000	-3.156578000	-1.462778000
C	1.601713000	-2.105762000	-2.405519000
C	2.789760000	-1.394220000	-2.015117000
C	-3.789763000	-1.208581000	0.032453000
C	-3.210383000	-2.535639000	0.177169000
C	-2.825204000	-2.724888000	1.540222000
C	-3.156157000	-1.531534000	2.263226000
C	-3.752176000	-0.605585000	1.355163000
H	-1.154296000	0.864561000	-0.015216000
C	5.831988000	-0.072765000	-0.567740000
H	6.768010000	0.056937000	-0.001822000
H	6.100775000	-0.178935000	-1.627578000
H	5.242047000	0.846391000	-0.450215000
C	6.077265000	-3.084658000	-0.027611000
H	7.027908000	-2.896278000	0.494778000
H	5.639101000	-3.996515000	0.403059000
H	6.313016000	-3.298361000	-1.080788000

C	4.607569000	-1.221706000	1.969240000
H	5.556871000	-0.953746000	2.459327000
H	3.918688000	-0.371217000	2.061821000
H	4.180181000	-2.068246000	2.524942000
C	3.385118000	-0.247702000	-2.800350000
H	3.727268000	0.557087000	-2.142135000
H	4.243312000	-0.587571000	-3.401846000
H	2.649460000	0.175532000	-3.496530000
C	0.774045000	-1.841344000	-3.640936000
H	0.714817000	-0.770058000	-3.871380000
H	1.207794000	-2.345216000	-4.519894000
H	-0.253613000	-2.206072000	-3.521977000
C	0.329155000	-4.221412000	-1.530319000
H	-0.520236000	-3.907814000	-2.147979000
H	0.732895000	-5.148342000	-1.970365000
H	-0.053223000	-4.473354000	-0.532268000
C	2.598227000	-4.083344000	0.639134000
H	3.160969000	-4.961664000	0.283536000
H	3.147850000	-3.663145000	1.489107000
H	1.631476000	-4.447062000	1.012601000
C	1.831907000	4.046538000	-2.826867000
H	1.631447000	4.354611000	-3.865085000
H	2.591173000	4.728759000	-2.422142000
H	2.265453000	3.037301000	-2.861373000
C	-0.452829000	5.884721000	-1.900281000
H	-0.574917000	6.233177000	-2.937295000
H	-1.428306000	5.979359000	-1.402029000
H	0.243866000	6.570857000	-1.396741000
C	-1.018358000	2.976789000	-2.811227000
H	-0.962765000	3.209182000	-3.886451000
H	-0.767991000	1.915017000	-2.678553000
H	-2.065326000	3.113278000	-2.505774000
C	-2.163521000	3.711850000	0.622532000
H	-2.384456000	4.786652000	0.730457000
H	-2.454328000	3.418320000	-0.392602000
H	-2.808070000	3.174631000	1.327742000
C	-0.967789000	3.067355000	3.470568000
H	-1.247624000	4.062091000	3.854185000
H	-1.896122000	2.502764000	3.312538000
H	-0.401240000	2.562186000	4.262945000
C	2.252054000	3.057650000	3.223124000
H	2.670377000	4.039923000	3.494110000
H	1.779231000	2.645754000	4.123066000
H	3.094584000	2.405763000	2.955272000
C	3.031213000	3.581793000	0.227103000
H	3.198963000	2.997277000	-0.683571000
H	3.280735000	4.633696000	0.015536000
H	3.739413000	3.217471000	0.980711000
C	-2.944369000	-1.320779000	3.742221000
H	-2.802970000	-0.260094000	3.985199000
H	-3.812467000	-1.678653000	4.319038000
H	-2.062713000	-1.865444000	4.103879000
C	-2.279923000	-3.992837000	2.145899000
H	-1.635068000	-3.784617000	3.009685000
H	-3.099318000	-4.640644000	2.496671000
H	-1.691113000	-4.569902000	1.421818000
C	-3.213328000	-3.626329000	-0.868777000
H	-4.191590000	-4.133819000	-0.884043000
H	-3.030439000	-3.238162000	-1.877263000
H	-2.454804000	-4.388926000	-0.660045000
C	-3.509178000	-0.692787000	-3.071679000
H	-3.296830000	-1.723081000	-3.390241000
H	-3.991833000	-0.185454000	-3.921627000
H	-2.547679000	-0.195346000	-2.883542000
C	-6.182937000	-1.683235000	-1.853003000
H	-6.882136000	-1.629137000	-1.005662000
H	-6.721525000	-1.347634000	-2.752485000

H	-5.922115000	-2.740780000	-1.999860000
C	-5.247705000	1.201772000	-1.434610000
H	-5.725809000	1.464465000	-2.391236000
H	-5.993614000	1.357252000	-0.643346000
H	-4.426542000	1.915068000	-1.276718000
C	-4.374212000	0.705235000	1.775605000
H	-4.292668000	1.472271000	1.001365000
H	-5.446441000	0.566722000	1.992928000
H	-3.905097000	1.093780000	2.688362000

G'

Ti	0.844471000	1.453237000	0.617202000
Ti	1.214847000	-1.070141000	-0.206933000
Ti	-1.596810000	-0.392882000	0.669008000
Si	0.583561000	4.078395000	-2.154590000
Si	4.362203000	-2.738876000	0.547042000
Si	-4.456270000	-1.418724000	-1.626677000
N	-0.294940000	0.351055000	-0.688508000
N	2.215581000	0.373135000	0.358919000
C	-0.065346000	-1.546712000	1.341949000
H	-0.109609000	-2.406116000	2.028970000
C	-0.148721000	-0.161063000	1.980570000
C	0.368297000	-0.006894000	3.398195000
H	0.133507000	-0.899735000	4.002632000
H	-0.059886000	0.869892000	3.903475000
H	1.467076000	0.101775000	3.416395000
C	0.787598000	3.670033000	-0.316645000
C	-0.218416000	3.708859000	0.722466000
C	0.410987000	3.487271000	1.983594000
C	1.824392000	3.334310000	1.750881000
C	2.059538000	3.469596000	0.351796000
C	2.913327000	-2.593277000	-0.671531000
C	1.707080000	-3.397596000	-0.610495000
C	0.861041000	-3.025853000	-1.693918000
C	1.514055000	-1.987804000	-2.435905000
C	2.786275000	-1.738169000	-1.831133000
C	-3.742130000	-1.106787000	0.099365000
C	-3.265275000	-2.055553000	1.092315000
C	-3.115230000	-1.383774000	2.341488000
C	-3.465508000	-0.011149000	2.161493000
C	-3.854123000	0.167223000	0.793344000
H	-0.522264000	0.590440000	-1.662407000
C	5.760187000	-1.501689000	0.200829000
H	6.569944000	-1.676261000	0.926677000
H	6.190967000	-1.603541000	-0.804397000
H	5.417958000	-0.465436000	0.326553000
C	5.088098000	-4.495148000	0.397284000
H	5.936439000	-4.625344000	1.086718000
H	4.348167000	-5.273527000	0.631751000
H	5.455175000	-4.685358000	-0.622196000
C	3.810410000	-2.434479000	2.342866000
H	4.680372000	-2.495337000	3.015953000
H	3.378568000	-1.427894000	2.434986000
H	3.062305000	-3.153115000	2.705257000
C	3.810019000	-0.758943000	-2.356579000
H	4.166199000	-0.085544000	-1.569518000
H	4.677940000	-1.288307000	-2.779343000
H	3.385510000	-0.140508000	-3.157263000
C	0.982499000	-1.376852000	-3.710845000
H	1.375454000	-0.367133000	-3.881772000
H	1.262289000	-1.988393000	-4.584022000
H	-0.114166000	-1.311950000	-3.701551000
C	-0.450313000	-3.664308000	-2.067844000
H	-1.202770000	-2.917612000	-2.355689000
H	-0.323955000	-4.344442000	-2.926259000
H	-0.858205000	-4.253761000	-1.238953000
C	1.417063000	-4.519915000	0.357715000

H	1.698003000	-5.493800000	-0.075146000
H	1.974504000	-4.402477000	1.293688000
H	0.350157000	-4.565979000	0.613372000
C	1.591825000	2.916582000	-3.282193000
H	1.174498000	2.938356000	-4.300972000
H	2.648323000	3.208345000	-3.358808000
H	1.559744000	1.877201000	-2.926901000
C	1.173250000	5.864893000	-2.445286000
H	1.089396000	6.143515000	-3.506858000
H	0.578249000	6.583053000	-1.862303000
H	2.224911000	5.991324000	-2.149658000
C	-1.221827000	3.950721000	-2.747825000
H	-1.247535000	4.130020000	-3.833977000
H	-1.650435000	2.952837000	-2.572198000
H	-1.883996000	4.690835000	-2.278980000
C	-1.682489000	4.038773000	0.557479000
H	-1.821328000	5.110323000	0.340914000
H	-2.151472000	3.478615000	-0.258728000
H	-2.237627000	3.824493000	1.479626000
C	-0.248972000	3.600454000	3.338038000
H	-0.403615000	4.658675000	3.604928000
H	-1.229200000	3.108009000	3.370878000
H	0.372314000	3.157503000	4.125979000
C	2.882671000	3.139078000	2.811171000
H	3.270183000	4.108402000	3.164760000
H	2.489233000	2.605712000	3.686657000
H	3.731341000	2.560686000	2.425684000
C	3.429792000	3.460850000	-0.283354000
H	3.399121000	3.106139000	-1.318440000
H	3.862926000	4.474835000	-0.285621000
H	4.115033000	2.803462000	0.265459000
C	-3.532961000	1.032884000	3.249053000
H	-3.422189000	2.047500000	2.845607000
H	-4.505481000	0.995566000	3.766437000
H	-2.750385000	0.885576000	4.003852000
C	-2.703896000	-2.028298000	3.639185000
H	-2.386250000	-1.281768000	4.376707000
H	-3.542640000	-2.592835000	4.076942000
H	-1.873404000	-2.733449000	3.497455000
C	-4.444655000	1.441337000	0.229645000
H	-4.256765000	1.546772000	-0.846486000
H	-5.536585000	1.457146000	0.374671000
H	-4.042287000	2.332520000	0.725930000
C	-3.064776000	-3.541965000	0.919200000
H	-4.000065000	-4.089324000	1.122029000
H	-2.746650000	-3.799354000	-0.094936000
H	-2.305322000	-3.919508000	1.616036000
C	-6.277062000	-0.857340000	-1.655939000
H	-6.395608000	0.225270000	-1.514767000
H	-6.735568000	-1.115322000	-2.623067000
H	-6.857515000	-1.360778000	-0.868842000
C	-4.477821000	-3.256057000	-2.117780000
H	-3.479105000	-3.689027000	-2.259507000
H	-5.013393000	-3.874007000	-1.383665000
H	-5.012467000	-3.349144000	-3.076053000
C	-3.513705000	-0.468474000	-2.983795000
H	-3.504539000	0.617745000	-2.811411000
H	-2.467410000	-0.800591000	-3.050725000
H	-3.979777000	-0.639641000	-3.966513000

TS10'

Ti	-0.638171000	1.301864000	-0.488800000
H	-2.075575000	0.285239000	0.005296000
Ti	1.727552000	-0.197728000	0.252942000
Ti	-0.939253000	-1.166414000	0.466811000
Si	-1.761390000	4.489720000	1.090093000
Si	5.229092000	-1.077763000	-1.148339000

Si	-4.006837000	-3.070467000	-1.029617000
N	0.861365000	-1.903674000	-0.045811000
N	0.041480000	0.421172000	1.017673000
C	-0.459220000	-0.542813000	-1.561082000
H	-0.927468000	-0.557407000	-2.551400000
C	0.667583000	-1.455511000	-1.386344000
C	1.065642000	-2.421911000	-2.500304000
H	1.183765000	-1.890450000	-3.453269000
H	0.272543000	-3.173707000	-2.616662000
H	1.999170000	-2.935519000	-2.248003000
C	-1.452424000	3.491867000	-0.495391000
C	-2.460038000	2.677640000	-1.142930000
C	-1.932070000	2.181298000	-2.379221000
C	-0.594808000	2.662118000	-2.514962000
C	-0.295583000	3.466551000	-1.365949000
C	4.105785000	-0.406529000	0.223766000
C	3.600704000	-1.111288000	1.379720000
C	2.988728000	-0.160356000	2.258321000
C	3.136655000	1.145186000	1.681397000
C	3.815640000	0.999759000	0.437151000
C	-2.853045000	-2.631521000	0.411944000
C	-1.721415000	-3.437172000	0.805522000
C	-1.217748000	-2.960723000	2.050960000
C	-2.036236000	-1.857530000	2.469816000
C	-3.044966000	-1.658605000	1.475190000
H	1.262157000	1.225673000	-0.845799000
H	1.958732000	-0.480212000	-1.492700000
C	3.736861000	-2.589041000	1.665192000
H	3.361198000	-3.202016000	0.838037000
H	4.789660000	-2.857610000	1.842745000
H	3.174827000	-2.867077000	2.564655000
C	2.374585000	-0.417266000	3.612600000
H	1.446133000	0.153986000	3.742052000
H	2.142639000	-1.477768000	3.762404000
H	3.067953000	-0.114682000	4.414027000
C	2.669178000	2.420420000	2.336171000
H	1.639219000	2.322877000	2.704937000
H	3.309728000	2.677334000	3.195112000
H	2.697843000	3.266993000	1.639938000
C	4.238795000	2.131573000	-0.470232000
H	5.334667000	2.242971000	-0.467843000
H	3.920511000	1.963311000	-1.505197000
H	3.811979000	3.085932000	-0.140855000
C	7.025444000	-0.643974000	-0.678506000
H	7.307353000	-1.097539000	0.283123000
H	7.731459000	-1.009790000	-1.439808000
H	7.173037000	0.441975000	-0.585333000
C	4.858735000	-0.325512000	-2.856554000
H	3.783306000	-0.354309000	-3.080673000
H	5.195337000	0.716805000	-2.941117000
H	5.384265000	-0.902764000	-3.633159000
C	5.135201000	-2.968695000	-1.333014000
H	5.526622000	-3.499436000	-0.454832000
H	4.112393000	-3.326267000	-1.513519000
H	5.747367000	-3.268449000	-2.197911000
C	-0.264902000	5.533167000	1.625258000
H	0.074204000	6.226058000	0.843055000
H	-0.561557000	6.139962000	2.495084000
H	0.592755000	4.920204000	1.934864000
C	-3.194213000	5.702033000	0.768923000
H	-4.131874000	5.187698000	0.517306000
H	-3.383511000	6.318325000	1.661149000
H	-2.956400000	6.382865000	-0.061626000
C	-2.204663000	3.361267000	2.557294000
H	-1.416485000	2.613933000	2.728014000
H	-2.313228000	3.959912000	3.475253000
H	-3.147683000	2.816844000	2.407047000

C	0.994891000	4.233821000	-1.197339000
H	0.872002000	5.274725000	-1.538202000
H	1.327345000	4.266009000	-0.155070000
H	1.797330000	3.781948000	-1.791533000
C	-3.898447000	2.509143000	-0.713075000
H	-4.013076000	2.561636000	0.375185000
H	-4.525841000	3.300645000	-1.154206000
H	-4.303549000	1.545184000	-1.043990000
C	-2.698736000	1.359206000	-3.383626000
H	-3.305349000	0.584567000	-2.896363000
H	-3.382492000	1.996046000	-3.967237000
H	-2.029261000	0.861420000	-4.096242000
C	0.337760000	2.402925000	-3.672098000
H	0.021705000	1.526627000	-4.251285000
H	0.365310000	3.264046000	-4.358997000
H	1.361822000	2.215003000	-3.325341000
C	-5.455213000	-1.856159000	-1.243051000
H	-6.083074000	-2.209966000	-2.075750000
H	-6.096226000	-1.793139000	-0.353375000
H	-5.123086000	-0.839243000	-1.495610000
C	-4.760180000	-4.778967000	-0.651223000
H	-5.448804000	-5.090298000	-1.451607000
H	-3.990175000	-5.557461000	-0.553925000
H	-5.329065000	-4.759878000	0.290072000
C	-3.127372000	-3.150375000	-2.715169000
H	-3.861126000	-3.388684000	-3.501258000
H	-2.664782000	-2.186113000	-2.965769000
H	-2.340160000	-3.915365000	-2.761085000
C	-4.189859000	-0.685596000	1.632269000
H	-4.508841000	-0.263981000	0.675818000
H	-5.059118000	-1.185380000	2.090852000
H	-3.908714000	0.147997000	2.287538000
C	-1.909722000	-1.097161000	3.768779000
H	-0.886472000	-1.141160000	4.160938000
H	-2.169378000	-0.038496000	3.646507000
H	-2.578704000	-1.519678000	4.535734000
C	-0.054142000	-3.573539000	2.786078000
H	0.243202000	-2.969591000	3.651561000
H	-0.316571000	-4.576774000	3.158201000
H	0.815095000	-3.680790000	2.123074000
C	-1.120736000	-4.614344000	0.076960000
H	-1.565998000	-4.755837000	-0.913630000
H	-0.037409000	-4.478610000	-0.051688000
H	-1.277114000	-5.542837000	0.648917000

J

Ti	-0.529031000	1.333392000	-0.492176000
H	-2.006626000	0.462148000	0.099457000
Ti	1.712773000	-0.303777000	0.353734000
Ti	-0.977287000	-1.118285000	0.480886000
Si	-1.504363000	4.546583000	1.107545000
Si	5.110673000	-1.189269000	-1.279789000
Si	-4.190980000	-2.822535000	-1.052894000
N	0.780081000	-1.928095000	0.002372000
N	0.126296000	0.433839000	1.047453000
C	-0.556692000	-0.529020000	-1.523611000
H	-1.146400000	-0.639446000	-2.439696000
C	0.672995000	-1.416519000	-1.409696000
C	0.828557000	-2.546493000	-2.439262000
H	0.887281000	-2.132429000	-3.456114000
H	-0.043279000	-3.208594000	-2.380236000
H	1.731566000	-3.135589000	-2.234351000
C	-1.243715000	3.553817000	-0.489345000
C	-2.287441000	2.791525000	-1.144178000
C	-1.778635000	2.271072000	-2.377413000
C	-0.419580000	2.690082000	-2.507646000
C	-0.087936000	3.479866000	-1.358272000

C	4.093308000	-0.610087000	0.215473000
C	3.593269000	-1.386359000	1.327382000
C	3.047232000	-0.483406000	2.297596000
C	3.233770000	0.859006000	1.823033000
C	3.873928000	0.786305000	0.552768000
C	-2.998148000	-2.449511000	0.373062000
C	-1.929030000	-3.335362000	0.773326000
C	-1.418700000	-2.915743000	2.034491000
C	-2.163818000	-1.762961000	2.455150000
C	-3.140834000	-1.482807000	1.448864000
H	1.386222000	1.116633000	-0.811986000
H	1.624474000	-0.749377000	-1.582005000
C	6.870294000	-0.483778000	-1.097410000
H	7.513233000	-0.829359000	-1.921346000
H	6.881943000	0.615067000	-1.107632000
H	7.332007000	-0.810717000	-0.154202000
C	4.395637000	-0.612089000	-2.948925000
H	5.092748000	-0.881318000	-3.758080000
H	3.435858000	-1.102382000	-3.164034000
H	4.230328000	0.472410000	-3.005037000
C	5.268353000	-3.080326000	-1.392636000
H	4.299918000	-3.578922000	-1.537811000
H	5.896301000	-3.324733000	-2.263680000
H	5.746855000	-3.522708000	-0.508584000
C	3.658339000	-2.886242000	1.493288000
H	3.319855000	-3.413253000	0.594947000
H	4.685835000	-3.211755000	1.718411000
H	3.022425000	-3.214621000	2.323728000
C	2.466086000	-0.833946000	3.645968000
H	2.128943000	-1.875558000	3.688500000
H	3.221531000	-0.698306000	4.436813000
H	1.610797000	-0.191194000	3.890755000
C	2.851889000	2.106610000	2.578691000
H	1.875163000	1.994713000	3.067243000
H	3.594108000	2.338271000	3.359699000
H	2.794059000	2.976625000	1.912988000
C	4.363240000	1.981291000	-0.230883000
H	5.378567000	2.261675000	0.092759000
H	4.402438000	1.779173000	-1.306899000
H	3.718091000	2.854287000	-0.080635000
C	0.049943000	5.486860000	1.670701000
H	0.437839000	6.173203000	0.905626000
H	-0.215075000	6.093042000	2.551116000
H	0.865242000	4.815299000	1.973992000
C	-2.857406000	5.849338000	0.794118000
H	-3.820990000	5.396144000	0.523324000
H	-3.020182000	6.460247000	1.695244000
H	-2.570086000	6.529007000	-0.021629000
C	-2.023892000	3.426717000	2.555471000
H	-1.291330000	2.620842000	2.706257000
H	-2.083936000	4.014700000	3.484780000
H	-3.004776000	2.955840000	2.400634000
C	1.236354000	4.183789000	-1.174812000
H	1.161115000	5.236622000	-1.491543000
H	1.569646000	4.178394000	-0.131824000
H	2.018359000	3.711085000	-1.780307000
C	0.492656000	2.389438000	-3.670599000
H	0.466620000	3.202694000	-4.414065000
H	1.532941000	2.267733000	-3.344313000
H	0.196948000	1.463208000	-4.178498000
C	-2.575138000	1.494783000	-3.393852000
H	-3.186882000	2.173161000	-4.010099000
H	-1.923154000	0.932271000	-4.073608000
H	-3.257126000	0.780109000	-2.915225000
C	-3.734851000	2.699125000	-0.722641000
H	-3.852453000	2.750948000	0.365118000
H	-4.314518000	3.526847000	-1.162718000

H	-4.190564000	1.761302000	-1.062106000
C	-5.565641000	-1.523357000	-1.261710000
H	-6.222588000	-1.845176000	-2.084957000
H	-6.192271000	-1.413909000	-0.366369000
H	-5.175423000	-0.530506000	-1.526806000
C	-3.357688000	-2.979426000	-2.756789000
H	-2.594275000	-3.768002000	-2.801707000
H	-4.121376000	-3.219844000	-3.513344000
H	-2.876079000	-2.037883000	-3.052753000
C	-5.046013000	-4.477611000	-0.649616000
H	-5.767794000	-4.750053000	-1.434904000
H	-4.324621000	-5.302538000	-0.560949000
H	-5.594470000	-4.417493000	0.302068000
C	-1.402600000	-4.544731000	0.040391000
H	-1.824549000	-4.631230000	-0.966781000
H	-0.308279000	-4.496710000	-0.051442000
H	-1.653593000	-5.467963000	0.587132000
C	-4.219649000	-0.436832000	1.603353000
H	-4.498464000	0.012823000	0.647164000
H	-5.125972000	-0.881030000	2.047455000
H	-3.891213000	0.370822000	2.269079000
C	-2.002677000	-1.026039000	3.764156000
H	-2.180595000	0.050350000	3.648871000
H	-2.713087000	-1.403372000	4.517416000
H	-0.991915000	-1.149859000	4.172524000
C	-0.306230000	-3.611129000	2.775403000
H	-0.629789000	-4.607108000	3.117698000
H	0.569021000	-3.750954000	2.125467000
H	0.006986000	-3.045293000	3.661067000

TS13

Ti	-0.412888000	1.262004000	-0.921832000
H	-1.914297000	0.489668000	-0.254774000
Ti	1.706519000	-0.281888000	0.341586000
Ti	-1.006017000	-1.070186000	0.479949000
Si	-1.533360000	4.118668000	1.440871000
Si	5.133776000	-1.175729000	-1.259458000
Si	-4.091673000	-2.796994000	-1.188813000
N	0.774319000	-1.945600000	0.159139000
N	0.094451000	0.526382000	0.821695000
C	-0.636133000	-0.938972000	-1.576957000
H	-1.283544000	-1.345359000	-2.361477000
C	0.684075000	-1.675673000	-1.306717000
C	0.981897000	-2.919232000	-2.160410000
H	1.059963000	-2.644188000	-3.222316000
H	0.166715000	-3.642458000	-2.044593000
H	1.917250000	-3.394828000	-1.838729000
C	-1.238058000	3.402649000	-0.291529000
C	-2.266963000	2.789428000	-1.099668000
C	-1.772999000	2.605727000	-2.430527000
C	-0.442086000	3.137287000	-2.478383000
C	-0.098863000	3.598583000	-1.169102000
C	4.103994000	-0.594486000	0.225723000
C	3.598756000	-1.363708000	1.340145000
C	3.035581000	-0.455913000	2.293613000
C	3.220873000	0.884537000	1.809782000
C	3.873791000	0.803925000	0.546773000
C	-2.979104000	-2.481705000	0.310864000
C	-1.920914000	-3.311332000	0.834899000
C	-1.514756000	-2.801479000	2.101622000
C	-2.327160000	-1.661090000	2.409773000
C	-3.230497000	-1.465827000	1.320648000
H	1.532893000	1.048904000	-0.917008000
H	1.558846000	-0.943345000	-1.566703000
H	0.417485000	1.018411000	-2.593772000
H	-0.010260000	0.244695000	-2.431404000
C	0.392807000	3.299909000	-3.725882000

H	0.228396000	4.298075000	-4.163482000
H	1.465494000	3.200428000	-3.518782000
H	0.127531000	2.556648000	-4.488156000
C	-2.536941000	2.071306000	-3.618178000
H	-2.899147000	2.894340000	-4.255554000
H	-1.911105000	1.423738000	-4.249001000
H	-3.410589000	1.487583000	-3.307338000
C	-3.700190000	2.557421000	-0.689877000
H	-3.793313000	2.397687000	0.388852000
H	-4.312346000	3.433545000	-0.958520000
H	-4.130022000	1.685656000	-1.195598000
C	1.196885000	4.302088000	-0.841717000
H	1.074888000	5.395106000	-0.913009000
H	1.541650000	4.073560000	0.171045000
H	1.989614000	4.012990000	-1.542127000
C	-2.930281000	5.409484000	1.308523000
H	-3.881935000	4.970111000	0.979147000
H	-3.106295000	5.882201000	2.287195000
H	-2.669436000	6.207011000	0.597027000
C	-0.028082000	5.043655000	2.145044000
H	0.823434000	4.381850000	2.350591000
H	0.318928000	5.858644000	1.495275000
H	-0.327909000	5.495562000	3.103692000
C	-2.016053000	2.792066000	2.706653000
H	-3.024209000	2.392354000	2.528189000
H	-1.307772000	1.954246000	2.654588000
H	-2.001460000	3.207125000	3.726398000
C	4.376940000	-0.668320000	-2.932505000
H	4.152619000	0.404951000	-3.000499000
H	5.076567000	-0.913489000	-3.747022000
H	3.440815000	-1.210868000	-3.127201000
C	5.371276000	-3.061377000	-1.317084000
H	6.022028000	-3.302987000	-2.172047000
H	5.856334000	-3.455670000	-0.413879000
H	4.429089000	-3.608066000	-1.459978000
C	6.870057000	-0.405804000	-1.114845000
H	7.516969000	-0.759782000	-1.932175000
H	6.849156000	0.691687000	-1.161558000
H	7.348422000	-0.687719000	-0.165373000
C	3.664672000	-2.861206000	1.520901000
H	4.686191000	-3.181706000	1.778623000
H	3.004282000	-3.184530000	2.334082000
H	3.354216000	-3.398574000	0.618488000
C	2.446307000	-0.800270000	3.640470000
H	2.060739000	-1.825310000	3.670109000
H	3.211160000	-0.711030000	4.429098000
H	1.624008000	-0.121842000	3.902896000
C	2.857325000	2.135768000	2.568155000
H	1.859098000	2.060501000	3.019081000
H	3.577287000	2.325985000	3.380680000
H	2.863609000	3.015749000	1.913985000
C	4.362336000	1.992881000	-0.246954000
H	5.369965000	2.289980000	0.085587000
H	4.417049000	1.774735000	-1.319446000
H	3.704844000	2.860264000	-0.119906000
C	-3.357522000	-3.995421000	-2.474036000
H	-3.277354000	-5.027436000	-2.105912000
H	-4.029636000	-4.014702000	-3.346450000
H	-2.367038000	-3.680496000	-2.832011000
C	-4.501479000	-1.195925000	-2.136704000
H	-4.804502000	-1.437649000	-3.167112000
H	-5.326423000	-0.630937000	-1.680277000
H	-3.622945000	-0.538972000	-2.186083000
C	-5.719916000	-3.566107000	-0.565516000
H	-6.410948000	-3.759996000	-1.400292000
H	-5.538863000	-4.522266000	-0.052747000
H	-6.235607000	-2.903602000	0.144881000

C	-1.302002000	-4.550114000	0.239307000
H	-1.549901000	-4.671952000	-0.818081000
H	-0.208014000	-4.512702000	0.333114000
H	-1.654455000	-5.449321000	0.771182000
C	-0.442273000	-3.413064000	2.965482000
H	-0.759595000	-4.397851000	3.344104000
H	0.484312000	-3.559723000	2.392402000
H	-0.216797000	-2.783636000	3.835047000
C	-2.305345000	-0.898662000	3.713464000
H	-2.896422000	-1.427599000	4.478764000
H	-1.285506000	-0.789630000	4.105893000
H	-2.726473000	0.106915000	3.606951000
C	-4.384441000	-0.492106000	1.339342000
H	-4.644037000	-0.141904000	0.336301000
H	-5.279647000	-0.968750000	1.772123000
H	-4.158404000	0.389259000	1.951762000

L

Ti	-0.126715000	1.340002000	-0.389114000
H	-1.782627000	0.607684000	-0.423886000
Ti	1.571689000	-0.856342000	0.416935000
Ti	-1.183769000	-1.198302000	-0.161685000
Si	-0.797948000	4.561136000	1.366482000
Si	4.958540000	-0.590240000	-1.356229000
Si	-5.082484000	-1.149301000	-0.678957000
N	0.602851000	-2.148568000	-0.437863000
N	0.074517000	0.105676000	0.977078000
C	-1.139985000	-2.181193000	-2.106277000
H	-1.884106000	-2.964920000	-2.282539000
C	0.258651000	-2.743044000	-1.768094000
C	0.365796000	-4.275022000	-1.775818000
H	0.152709000	-4.655020000	-2.785959000
H	-0.354242000	-4.723408000	-1.080412000
H	1.372464000	-4.603095000	-1.482295000
C	-0.553357000	3.627887000	-0.269838000
C	-1.541281000	3.071361000	-1.172427000
C	-0.871992000	2.578347000	-2.340939000
C	0.526234000	2.844943000	-2.198316000
C	0.728044000	3.487386000	-0.939340000
C	3.986019000	-0.858082000	0.250944000
C	3.581689000	-2.157518000	0.725556000
C	2.966372000	-2.005791000	2.007489000
C	3.020689000	-0.613304000	2.367477000
C	3.645207000	0.088826000	1.299112000
C	-3.553042000	-1.622186000	0.339633000
C	-2.917207000	-2.917775000	0.254302000
C	-1.940109000	-3.024222000	1.288324000
C	-1.965609000	-1.803680000	2.038297000
C	-2.954520000	-0.948530000	1.466031000
H	1.584002000	0.628707000	-0.763990000
H	1.004682000	-2.346795000	-2.475618000
H	-0.348199000	0.030628000	-1.517040000
H	-1.118718000	-1.500289000	-2.964160000
C	-5.894056000	0.483255000	-0.134244000
H	-6.833161000	0.601508000	-0.697506000
H	-6.152501000	0.483927000	0.934011000
H	-5.280325000	1.370185000	-0.336126000
C	-6.427126000	-2.475501000	-0.411920000
H	-7.352820000	-2.175738000	-0.927406000
H	-6.144389000	-3.465451000	-0.793324000
H	-6.664938000	-2.586386000	0.656448000
C	-4.697326000	-1.022569000	-2.536412000
H	-3.906313000	-0.283527000	-2.724211000
H	-4.351557000	-1.975748000	-2.959927000
H	-5.594021000	-0.713877000	-3.095793000
C	-3.355969000	-4.061706000	-0.626179000
H	-4.094053000	-4.684253000	-0.095447000

H	-3.826190000	-3.710109000	-1.551959000
H	-2.520140000	-4.713196000	-0.908462000
C	-1.116203000	-4.240437000	1.634582000
H	-1.456371000	-5.121877000	1.076771000
H	-0.052741000	-4.088390000	1.404257000
H	-1.202377000	-4.474902000	2.705953000
C	-1.192721000	-1.531221000	3.301529000
H	-1.804398000	-1.770818000	4.187365000
H	-0.285478000	-2.144712000	3.348599000
H	-0.888389000	-0.480245000	3.366463000
C	-3.306387000	0.399991000	2.042533000
H	-3.755047000	1.058217000	1.294105000
H	-4.022241000	0.295415000	2.874674000
H	-2.409305000	0.895537000	2.436409000
C	-2.611575000	4.638904000	1.929712000
H	-2.658604000	5.240090000	2.851248000
H	-3.268328000	5.119384000	1.191815000
H	-3.027722000	3.649803000	2.165986000
C	-0.207223000	6.356974000	1.141831000
H	-0.370370000	6.932043000	2.066142000
H	0.861986000	6.421617000	0.897469000
H	-0.762811000	6.858198000	0.335695000
C	0.182031000	3.750580000	2.784235000
H	-0.049850000	4.251739000	3.736967000
H	-0.079167000	2.687474000	2.888555000
H	1.270464000	3.811078000	2.641594000
C	2.042895000	4.071545000	-0.481443000
H	2.134291000	5.113743000	-0.827056000
H	2.141709000	4.077874000	0.609974000
H	2.895423000	3.517996000	-0.891944000
C	1.576504000	2.550636000	-3.239197000
H	1.601333000	3.345224000	-4.002318000
H	2.577123000	2.482386000	-2.797903000
H	1.375332000	1.602968000	-3.754876000
C	-1.530940000	1.979207000	-3.557999000
H	-1.872598000	2.768452000	-4.247342000
H	-0.837512000	1.332688000	-4.109373000
H	-2.403172000	1.372414000	-3.288538000
C	-3.043241000	3.125917000	-1.032834000
H	-3.371602000	2.980849000	0.000087000
H	-3.424082000	4.104134000	-1.369089000
H	-3.519975000	2.356181000	-1.650521000
C	5.536750000	1.203877000	-1.611641000
H	6.140086000	1.579177000	-0.773609000
H	6.168738000	1.238184000	-2.512829000
H	4.705101000	1.903450000	-1.772502000
C	6.538814000	-1.651954000	-1.291301000
H	6.325002000	-2.726682000	-1.215573000
H	7.141761000	-1.497245000	-2.199317000
H	7.162256000	-1.376904000	-0.427677000
C	3.934158000	-1.075795000	-2.884698000
H	3.006307000	-0.487827000	-2.933296000
H	4.505286000	-0.882824000	-3.806196000
H	3.652656000	-2.138315000	-2.889835000
C	3.986134000	1.556805000	1.348374000
H	5.000622000	1.706935000	1.753216000
H	3.953442000	2.019453000	0.359497000
H	3.293213000	2.103585000	2.000601000
C	2.571786000	-0.021846000	3.681750000
H	3.411109000	0.030935000	4.394155000
H	2.177761000	0.994360000	3.557063000
H	1.782780000	-0.625089000	4.147144000
C	2.532027000	-3.139430000	2.904118000
H	3.399225000	-3.545254000	3.450407000
H	1.801004000	-2.815177000	3.654586000
H	2.089223000	-3.965567000	2.334456000
C	3.812196000	-3.490873000	0.055472000

H	3.905512000	-3.395233000	-1.032542000
H	4.737472000	-3.959548000	0.428101000
H	2.986023000	-4.184323000	0.256637000

TS14

Ti	0.146429000	1.475688000	-0.413477000
H	-1.544621000	1.513315000	0.167602000
Ti	1.057413000	-1.379613000	0.380291000
Ti	-1.588517000	-0.380654000	0.407031000
Si	1.924819000	4.283336000	1.253447000
Si	4.382133000	-2.261299000	-1.396735000
Si	-5.062990000	-1.085562000	-1.203814000
N	-0.668962000	-2.068394000	-0.012399000
N	0.329825000	0.231657000	0.971431000
C	-0.766617000	-0.134263000	-1.586086000
H	-1.189536000	0.139882000	-2.559333000
C	-0.405791000	-1.609718000	-1.422886000
C	-0.926291000	-2.596453000	-2.474882000
H	-0.547521000	-2.331673000	-3.472393000
H	-2.022143000	-2.564942000	-2.494161000
H	-0.612826000	-3.617844000	-2.227701000
C	1.118327000	3.579757000	-0.315175000
C	-0.275263000	3.785847000	-0.662357000
C	-0.507156000	3.256473000	-1.973218000
C	0.722071000	2.714151000	-2.454158000
C	1.722782000	2.898915000	-1.445619000
C	3.248480000	-2.309309000	0.125235000
C	2.336241000	-3.401180000	0.415170000
C	1.785740000	-3.216033000	1.714320000
C	2.355423000	-2.013395000	2.268294000
C	3.262079000	-1.471122000	1.307258000
C	-3.946134000	-0.781248000	0.297835000
C	-3.367989000	-1.751681000	1.210618000
C	-2.841517000	-1.057791000	2.343201000
C	-3.082252000	0.343785000	2.162874000
C	-3.776707000	0.511955000	0.927705000
H	0.714304000	0.231271000	-1.526111000
H	0.780004000	-1.649359000	-1.544431000
C	5.367968000	-3.890809000	-1.445597000
H	6.069101000	-3.890917000	-2.294259000
H	5.958266000	-4.020909000	-0.526534000
H	4.722115000	-4.773319000	-1.550676000
C	5.661966000	-0.856388000	-1.338105000
H	6.348782000	-0.979646000	-2.190098000
H	5.210266000	0.140738000	-1.426198000
H	6.269671000	-0.875226000	-0.422955000
C	3.419601000	-2.070907000	-3.028062000
H	2.856415000	-1.126340000	-3.037274000
H	4.115816000	-2.060779000	-3.881477000
H	2.701028000	-2.885142000	-3.199999000
C	4.088372000	-0.228888000	1.536733000
H	5.099665000	-0.485854000	1.890806000
H	4.199438000	0.362177000	0.621659000
H	3.627668000	0.412692000	2.297968000
C	1.999467000	-4.570017000	-0.480798000
H	2.193835000	-4.347372000	-1.537145000
H	2.598374000	-5.455975000	-0.215128000
H	0.940937000	-4.847611000	-0.385426000
C	0.835508000	-4.167122000	2.398291000
H	0.016732000	-4.463791000	1.729322000
H	1.361621000	-5.082497000	2.713306000
H	0.393174000	-3.719318000	3.296082000
C	2.100663000	-1.468635000	3.653247000
H	2.866604000	-1.824964000	4.360626000
H	2.116582000	-0.371820000	3.666159000
H	1.123904000	-1.787652000	4.036822000
C	3.182725000	2.561055000	-1.639094000

H	3.740419000	3.435830000	-2.013289000
H	3.660836000	2.241788000	-0.708043000
H	3.304178000	1.753979000	-2.371854000
C	0.939472000	2.105881000	-3.817065000
H	1.273611000	2.869472000	-4.537688000
H	1.700728000	1.315938000	-3.791789000
H	0.015735000	1.664541000	-4.213395000
C	-1.807949000	3.306216000	-2.734666000
H	-1.851879000	4.196175000	-3.383124000
H	-1.936251000	2.426403000	-3.379141000
H	-2.668803000	3.348562000	-2.056359000
C	-1.289829000	4.571681000	0.135173000
H	-1.119854000	4.487116000	1.215160000
H	-1.242826000	5.641471000	-0.124941000
H	-2.310992000	4.228860000	-0.069320000
C	1.681154000	6.172545000	1.264446000
H	0.622269000	6.462692000	1.299295000
H	2.174393000	6.615582000	2.143306000
H	2.122140000	6.633176000	0.368168000
C	3.800998000	3.983097000	1.333353000
H	4.061816000	2.921823000	1.443916000
H	4.331822000	4.375664000	0.455140000
H	4.195460000	4.508716000	2.217128000
C	1.169838000	3.542189000	2.835321000
H	0.114959000	3.818541000	2.974415000
H	1.219093000	2.444129000	2.815520000
H	1.721214000	3.897299000	3.720167000
C	-4.505392000	-0.166015000	-2.774832000
H	-5.219506000	-0.361197000	-3.590414000
H	-4.448424000	0.922799000	-2.640514000
H	-3.514909000	-0.507606000	-3.105320000
C	-5.211178000	-2.922937000	-1.676599000
H	-5.597096000	-3.541245000	-0.854840000
H	-5.922820000	-3.006205000	-2.513073000
H	-4.262040000	-3.363548000	-2.011492000
C	-6.822409000	-0.500001000	-0.762088000
H	-7.519425000	-0.714587000	-1.586805000
H	-7.197904000	-1.015221000	0.134301000
H	-6.867408000	0.580307000	-0.565518000
C	-4.337937000	1.823066000	0.435315000
H	-4.366655000	1.871851000	-0.659341000
H	-5.367323000	1.961568000	0.803231000
H	-3.743495000	2.671433000	0.793601000
C	-3.360979000	-3.252116000	1.054954000
H	-4.335251000	-3.681341000	1.339010000
H	-3.139445000	-3.553294000	0.026413000
H	-2.597103000	-3.707549000	1.695969000
C	-2.193503000	-1.674348000	3.558085000
H	-2.938164000	-1.840375000	4.353767000
H	-1.738789000	-2.644382000	3.326712000
H	-1.411771000	-1.023404000	3.971001000
C	-2.713004000	1.432652000	3.139598000
H	-2.581898000	2.396778000	2.633030000
H	-3.496387000	1.560256000	3.904417000
H	-1.774426000	1.204034000	3.660731000

M

Ti	0.220423000	1.568018000	-0.568316000
H	-1.552507000	1.636419000	-0.204762000
Ti	0.909233000	-1.487210000	0.440309000
Ti	-1.565305000	-0.213862000	0.177893000
Si	1.176028000	4.663146000	1.349301000
Si	4.376741000	-2.393444000	-1.083679000
Si	-4.913676000	-1.709835000	-1.056107000
N	-0.759814000	-1.919810000	-0.426369000
N	0.255558000	0.262265000	0.812326000
C	-0.708097000	-0.071858000	-1.980632000

H	-1.773087000	-0.130421000	-2.297017000
C	-0.182266000	-1.495708000	-1.706720000
C	-0.342237000	-2.529044000	-2.835535000
H	0.201747000	-2.209006000	-3.736109000
H	-1.406724000	-2.622993000	-3.087854000
H	0.027697000	-3.514256000	-2.522639000
C	0.921746000	3.808098000	-0.325255000
C	-0.221246000	3.841242000	-1.210140000
C	0.110236000	3.151192000	-2.418021000
C	1.461162000	2.673211000	-2.310309000
C	1.959744000	3.083491000	-1.032509000
C	3.106490000	-2.390828000	0.324790000
C	2.176036000	-3.483960000	0.565397000
C	1.567109000	-3.299650000	1.841729000
C	2.125274000	-2.107942000	2.429696000
C	3.071616000	-1.561627000	1.515033000
C	-3.871150000	-0.885462000	0.295518000
C	-3.173448000	-1.567622000	1.365613000
C	-2.676124000	-0.590294000	2.281850000
C	-3.062465000	0.705459000	1.805643000
C	-3.807029000	0.526564000	0.595501000
H	-0.186356000	0.414062000	-2.818802000
H	0.968337000	-1.370278000	-1.581084000
C	5.362044000	-4.020332000	-0.981169000
H	4.727820000	-4.906556000	-1.120217000
H	6.144426000	-4.047758000	-1.755075000
H	5.856615000	-4.118465000	-0.003563000
C	5.650121000	-0.985215000	-0.962003000
H	6.403815000	-1.133828000	-1.751077000
H	5.211246000	0.010064000	-1.117402000
H	6.180621000	-0.974136000	-0.000184000
C	3.591851000	-2.266356000	-2.814183000
H	3.079235000	-1.303074000	-2.951033000
H	4.375889000	-2.336682000	-3.584434000
H	2.861189000	-3.061288000	-3.018065000
C	1.914227000	-4.671574000	-0.333369000
H	2.199039000	-4.469286000	-1.372951000
H	2.488481000	-5.551690000	-0.000997000
H	0.852069000	-4.951980000	-0.329189000
C	0.612078000	-4.264246000	2.502483000
H	-0.082603000	-4.707186000	1.777678000
H	1.164317000	-5.090105000	2.980383000
H	0.014983000	-3.777718000	3.283710000
C	1.832896000	-1.572884000	3.811005000
H	0.888934000	-1.966185000	4.206175000
H	2.629198000	-1.861269000	4.515843000
H	1.765790000	-0.477104000	3.817723000
C	3.894905000	-0.329206000	1.803747000
H	4.855892000	-0.597532000	2.272418000
H	4.118036000	0.240201000	0.896350000
H	3.368264000	0.339247000	2.496344000
C	3.383765000	2.877117000	-0.568607000
H	4.029759000	3.694622000	-0.927700000
H	3.462457000	2.849566000	0.524113000
H	3.804131000	1.939997000	-0.956578000
C	2.254591000	2.005121000	-3.407748000
H	2.686104000	2.752802000	-4.093845000
H	3.086388000	1.413649000	-3.004825000
H	1.632867000	1.332062000	-4.014497000
C	-0.779963000	3.020495000	-3.630804000
H	-0.770932000	3.947471000	-4.226479000
H	-0.448113000	2.208581000	-4.290904000
H	-1.823439000	2.817433000	-3.354740000
C	-1.534306000	4.555179000	-0.986919000
H	-1.871710000	4.483729000	0.051431000
H	-1.444529000	5.624717000	-1.237863000
H	-2.322070000	4.133564000	-1.623232000

C	1.640724000	3.428214000	2.722668000
H	2.641385000	2.994359000	2.585122000
H	1.635496000	3.934667000	3.700697000
H	0.925578000	2.594411000	2.763016000
C	2.576179000	5.941529000	1.162861000
H	2.323448000	6.696511000	0.403850000
H	2.746622000	6.469084000	2.113900000
H	3.528418000	5.480393000	0.865859000
C	-0.357266000	5.610798000	1.955183000
H	-0.711025000	6.358749000	1.232631000
H	-1.198053000	4.947200000	2.200053000
H	-0.087093000	6.147510000	2.878143000
C	-1.948999000	-0.834842000	3.580616000
H	-1.547701000	-1.853303000	3.633887000
H	-1.110569000	-0.138300000	3.708054000
H	-2.629042000	-0.699814000	4.437417000
C	-3.015655000	-3.059781000	1.514119000
H	-3.992240000	-3.564606000	1.492984000
H	-2.392234000	-3.468806000	0.707022000
H	-2.539681000	-3.311245000	2.469704000
C	-2.787393000	2.003494000	2.521537000
H	-3.531465000	2.181569000	3.315299000
H	-1.795628000	1.995510000	2.992059000
H	-2.819941000	2.856941000	1.834220000
C	-4.467006000	1.641933000	-0.183055000
H	-4.256331000	1.580765000	-1.257303000
H	-5.561198000	1.610519000	-0.056380000
H	-4.120707000	2.622007000	0.164655000
C	-6.691928000	-1.880206000	-0.393016000
H	-7.347395000	-2.361306000	-1.135110000
H	-6.719878000	-2.489737000	0.522128000
H	-7.127395000	-0.900079000	-0.148780000
C	-4.270808000	-3.437145000	-1.522744000
H	-4.501850000	-4.192342000	-0.759453000
H	-4.745643000	-3.761895000	-2.461621000
H	-3.182963000	-3.437815000	-1.673140000
C	-4.992513000	-0.694493000	-2.667133000
H	-5.563652000	0.237123000	-2.556689000
H	-3.996224000	-0.436695000	-3.054964000
H	-5.496897000	-1.296046000	-3.439448000

TS15

Ti	0.563720000	1.366644000	-0.525295000
H	-1.237555000	1.036234000	-0.884501000
Ti	0.986374000	-1.303506000	0.451100000
Ti	-1.611319000	-0.256553000	0.397145000
Si	1.792426000	4.389297000	1.209475000
Si	4.084742000	-2.883226000	-1.182179000
Si	-5.118411000	-1.196635000	-1.142234000
N	-0.766191000	-1.954178000	0.001608000
N	0.199905000	0.340904000	0.998491000
C	-0.904655000	0.022612000	-1.634073000
H	-1.404477000	0.232290000	-2.579989000
C	-0.506083000	-1.453963000	-1.395046000
C	-1.049465000	-2.426537000	-2.456910000
H	-0.702482000	-2.134589000	-3.458187000
H	-2.144828000	-2.406778000	-2.440572000
H	-0.712145000	-3.447511000	-2.241661000
C	1.318736000	3.515418000	-0.405793000
C	0.072495000	3.577284000	-1.155204000
C	0.262682000	2.903731000	-2.404845000
C	1.606840000	2.419587000	-2.458847000
C	2.262689000	2.789873000	-1.245572000
C	2.986977000	-2.609187000	0.340137000
C	1.906649000	-3.494162000	0.725600000
C	1.391445000	-3.071693000	1.983540000
C	2.159846000	-1.932410000	2.421359000

C	3.143067000	-1.658341000	1.425424000
C	-4.007354000	-0.517818000	0.233220000
C	-3.514352000	-1.228836000	1.392336000
C	-2.965844000	-0.270547000	2.309173000
C	-3.136920000	1.040690000	1.747706000
C	-3.769582000	0.889924000	0.478515000
H	1.829345000	-0.060536000	-0.691207000
H	0.647702000	-1.479548000	-1.525080000
C	3.115490000	-2.759318000	-2.816679000
H	3.782211000	-2.969881000	-3.667695000
H	2.274073000	-3.463819000	-2.877650000
H	2.711257000	-1.745378000	-2.949776000
C	5.526604000	-1.651282000	-1.313970000
H	6.167358000	-1.646008000	-0.421776000
H	6.155644000	-1.944206000	-2.169104000
H	5.188380000	-0.621889000	-1.495387000
C	4.853992000	-4.620724000	-1.045555000
H	4.095387000	-5.415096000	-1.015945000
H	5.512777000	-4.822355000	-1.904115000
H	5.460448000	-4.710360000	-0.132157000
C	1.379823000	-4.688432000	-0.034164000
H	1.684909000	-4.672573000	-1.087179000
H	1.754069000	-5.627953000	0.403453000
H	0.282197000	-4.718156000	-0.002649000
C	0.282251000	-3.757639000	2.740338000
H	-0.547263000	-4.023356000	2.072404000
H	0.647418000	-4.684990000	3.210583000
H	-0.115440000	-3.120774000	3.540021000
C	1.992638000	-1.215774000	3.739710000
H	0.950341000	-1.241325000	4.081258000
H	2.609774000	-1.687162000	4.521574000
H	2.288570000	-0.162405000	3.669557000
C	4.186512000	-0.573583000	1.539484000
H	5.147041000	-0.990002000	1.883390000
H	4.362537000	-0.072329000	0.582961000
H	3.881957000	0.188493000	2.266654000
C	3.730471000	2.570825000	-0.964024000
H	3.939678000	2.526253000	0.110796000
H	4.089214000	1.635198000	-1.411445000
H	4.334507000	3.391156000	-1.385227000
C	2.226077000	1.666542000	-3.609909000
H	2.631461000	2.360684000	-4.363945000
H	3.051187000	1.026588000	-3.273684000
H	1.490712000	1.025265000	-4.113501000
C	-0.749506000	2.809965000	-3.518783000
H	-0.741846000	3.726357000	-4.130783000
H	-0.535026000	1.966570000	-4.187173000
H	-1.770811000	2.682354000	-3.135658000
C	-1.155273000	4.391609000	-0.819147000
H	-1.420914000	4.331819000	0.240555000
H	-0.991361000	5.455773000	-1.058453000
H	-2.020471000	4.055248000	-1.402691000
C	3.143982000	5.675070000	0.824415000
H	2.788554000	6.415623000	0.092863000
H	3.433411000	6.219034000	1.736637000
H	4.052146000	5.213308000	0.412372000
C	2.443650000	3.177561000	2.525264000
H	3.406935000	2.724844000	2.251111000
H	2.590852000	3.705410000	3.480629000
H	1.726990000	2.360509000	2.690597000
C	0.344122000	5.324805000	2.012375000
H	-0.087308000	6.093887000	1.357449000
H	-0.465675000	4.655285000	2.334218000
H	0.721901000	5.834542000	2.912584000
C	-5.012141000	-3.086393000	-1.337859000
H	-5.407022000	-3.618733000	-0.462047000
H	-5.621658000	-3.384843000	-2.205160000

H	-3.989186000	-3.445644000	-1.513859000
C	-4.766511000	-0.431638000	-2.850429000
H	-5.344322000	-0.971755000	-3.616574000
H	-5.060049000	0.625388000	-2.906871000
H	-3.704555000	-0.500764000	-3.123267000
C	-6.920645000	-0.784138000	-0.676334000
H	-7.083164000	0.299468000	-0.582163000
H	-7.620430000	-1.159265000	-1.438922000
H	-7.196851000	-1.242382000	0.284625000
C	-4.198541000	2.024650000	-0.423063000
H	-3.824681000	1.901725000	-1.447295000
H	-5.296825000	2.084856000	-0.477873000
H	-3.836492000	2.988564000	-0.048270000
C	-2.761443000	2.322702000	2.449216000
H	-2.762937000	3.176766000	1.762288000
H	-3.474150000	2.548192000	3.259096000
H	-1.761271000	2.257501000	2.898557000
C	-2.394161000	-0.541979000	3.680863000
H	-1.545342000	0.118893000	3.899777000
H	-3.156718000	-0.372759000	4.458628000
H	-2.048228000	-1.577385000	3.782119000
C	-3.605154000	-2.714152000	1.654323000
H	-4.644071000	-3.017345000	1.858746000
H	-3.235839000	-3.301119000	0.806048000
H	-3.007640000	-2.992980000	2.530744000
N			
Ti	0.436319000	1.349516000	-0.534744000
H	-1.897057000	-0.211335000	-2.043956000
Ti	1.043184000	-1.260175000	0.457922000
Ti	-1.562798000	-0.309310000	0.259644000
Si	1.475026000	4.493471000	1.166566000
Si	4.276906000	-2.619702000	-1.150972000
Si	-5.037306000	-1.548541000	-0.998646000
N	-0.665751000	-2.027973000	-0.017233000
N	0.132708000	0.322883000	1.012686000
C	-0.810096000	-0.240149000	-1.788650000
H	-0.284716000	0.108525000	-2.687181000
C	-0.345299000	-1.689734000	-1.431501000
C	-0.759739000	-2.801702000	-2.411080000
H	-0.382738000	-2.585994000	-3.421187000
H	-1.854528000	-2.858953000	-2.452124000
H	-0.374506000	-3.774405000	-2.081444000
C	1.004188000	3.558914000	-0.412871000
C	-0.260060000	3.552044000	-1.139754000
C	-0.057753000	2.906785000	-2.395451000
C	1.312563000	2.500605000	-2.484416000
C	1.973623000	2.894262000	-1.277596000
C	3.146631000	-2.406806000	0.358159000
C	2.138545000	-3.369337000	0.756337000
C	1.592759000	-2.970469000	2.008890000
C	2.271240000	-1.768669000	2.430986000
C	3.230308000	-1.433880000	1.430596000
C	-3.920736000	-0.705921000	0.277594000
C	-3.335025000	-1.315021000	1.455774000
C	-2.814218000	-0.273428000	2.286868000
C	-3.092433000	0.988675000	1.659601000
C	-3.769790000	0.730199000	0.434300000
H	1.814010000	0.046845000	-0.679105000
H	0.798921000	-1.599280000	-1.531193000
C	5.169878000	-4.293949000	-0.983940000
H	4.472626000	-5.142804000	-0.958347000
H	5.855682000	-4.452956000	-1.830205000
H	5.766714000	-4.329660000	-0.060605000
C	5.624409000	-1.285831000	-1.286569000
H	6.279547000	-1.540743000	-2.134283000
H	5.213513000	-0.285634000	-1.480943000

H	6.256558000	-1.224606000	-0.390393000
C	3.320400000	-2.590280000	-2.797776000
H	2.854363000	-1.606926000	-2.957526000
H	4.010122000	-2.773156000	-3.636639000
H	2.527328000	-3.349057000	-2.854922000
C	1.716956000	-4.618041000	0.019711000
H	2.006871000	-4.589894000	-1.037504000
H	2.182694000	-5.512048000	0.464943000
H	0.627584000	-4.751619000	0.067296000
C	0.537405000	-3.725597000	2.776864000
H	-0.257370000	-4.083368000	2.110111000
H	0.975833000	-4.601052000	3.282630000
H	0.074573000	-3.099478000	3.549459000
C	2.060140000	-1.052110000	3.742950000
H	1.037979000	-1.189465000	4.115959000
H	2.748644000	-1.436819000	4.512596000
H	2.232047000	0.026572000	3.647892000
C	4.186694000	-0.270699000	1.531954000
H	5.177705000	-0.608481000	1.875572000
H	4.320027000	0.235999000	0.571391000
H	3.825631000	0.470098000	2.255101000
C	3.461877000	2.778765000	-1.044196000
H	3.994824000	3.638979000	-1.482528000
H	3.708506000	2.748463000	0.023498000
H	3.869258000	1.869636000	-1.505075000
C	1.968881000	1.824707000	-3.664370000
H	2.430198000	2.565935000	-4.337244000
H	2.760928000	1.134414000	-3.345713000
H	1.247460000	1.251710000	-4.262999000
C	-1.093057000	2.752319000	-3.481880000
H	-1.132297000	3.653440000	-4.114834000
H	-0.871590000	1.903584000	-4.142666000
H	-2.097432000	2.597054000	-3.067594000
C	-1.515740000	4.307514000	-0.778991000
H	-1.736072000	4.267626000	0.291152000
H	-1.415565000	5.371528000	-1.053804000
H	-2.383381000	3.911505000	-1.318957000
C	0.020714000	5.425744000	1.964063000
H	0.408032000	5.983892000	2.830976000
H	-0.441373000	6.155272000	1.285037000
H	-0.768170000	4.757210000	2.334801000
C	2.782238000	5.809674000	0.729895000
H	3.055152000	6.392503000	1.623173000
H	3.705060000	5.368681000	0.328472000
H	2.397517000	6.513754000	-0.022650000
C	2.186650000	3.343199000	2.506078000
H	1.485145000	2.528437000	2.735162000
H	3.139526000	2.884472000	2.206353000
H	2.372237000	3.909127000	3.432483000
C	-4.329150000	1.777193000	-0.502299000
H	-3.894346000	1.718332000	-1.509288000
H	-5.418506000	1.660867000	-0.610274000
H	-4.142891000	2.787418000	-0.121018000
C	-2.760617000	2.318970000	2.285920000
H	-3.095305000	3.156664000	1.664200000
H	-3.252548000	2.417407000	3.266485000
H	-1.678615000	2.425806000	2.447110000
C	-2.162108000	-0.412241000	3.641418000
H	-1.303464000	0.264555000	3.739502000
H	-2.876149000	-0.167658000	4.444916000
H	-1.805989000	-1.433784000	3.820418000
C	-3.321569000	-2.785259000	1.801217000
H	-4.340328000	-3.155589000	1.993675000
H	-2.878808000	-3.386589000	0.998584000
H	-2.733772000	-2.965729000	2.709306000
C	-6.845713000	-1.252847000	-0.473647000
H	-7.544047000	-1.735331000	-1.174645000

H	-7.038196000	-1.665565000	0.527484000
H	-7.095614000	-0.182403000	-0.440362000
C	-4.824248000	-0.864884000	-2.764851000
H	-5.063503000	0.203971000	-2.844347000
H	-3.805088000	-1.011161000	-3.151202000
H	-5.508003000	-1.403048000	-3.439964000
C	-4.773322000	-3.429149000	-1.107205000
H	-3.724670000	-3.700959000	-1.289596000
H	-5.099974000	-3.952018000	-0.198398000
H	-5.369739000	-3.822331000	-1.945319000

TS11'

Ti	-0.451009000	1.365184000	-0.671840000
H	-1.759016000	0.029531000	-0.697179000
Ti	1.790645000	-0.155250000	-0.021689000
Ti	-0.833729000	-1.298738000	0.389006000
Si	-1.403239000	4.422000000	1.379073000
Si	5.212465000	-1.406055000	-1.021164000
Si	-4.361975000	-2.579931000	-0.934118000
N	0.923026000	-1.859055000	-0.311623000
N	0.021298000	0.389943000	0.799840000
C	0.315302000	-0.375828000	-2.209061000
H	-0.643250000	0.163752000	-2.430046000
C	0.091817000	-1.707490000	-1.486377000
C	0.043110000	-2.907477000	-2.424482000
H	-0.796159000	-2.825440000	-3.129250000
H	-0.045576000	-3.851061000	-1.877371000
H	0.971194000	-2.960552000	-3.025446000
C	-1.167253000	3.560722000	-0.302289000
C	-2.233061000	2.886407000	-1.016916000
C	-1.782890000	2.569614000	-2.337488000
C	-0.432709000	3.029155000	-2.464113000
C	-0.052911000	3.641363000	-1.225584000
C	4.102399000	-0.606627000	0.292858000
C	3.392532000	-1.334342000	1.320317000
C	2.737086000	-0.393789000	2.167673000
C	3.068770000	0.928957000	1.711380000
C	3.916534000	0.803912000	0.576294000
C	-3.021577000	-2.447904000	0.399557000
C	-2.019525000	-3.457057000	0.639316000
C	-1.333949000	-3.159526000	1.854181000
C	-1.924871000	-1.970174000	2.411139000
C	-2.953571000	-1.535556000	1.522818000
H	0.748228000	-0.491601000	-3.224207000
H	1.367978000	1.581748000	-0.706016000
H	1.613631000	0.133630000	-1.934679000
H	2.578223000	0.213206000	-1.648219000
C	6.851321000	-1.904587000	-0.184571000
H	6.689178000	-2.605391000	0.647381000
H	7.527630000	-2.392920000	-0.902804000
H	7.374749000	-1.026966000	0.222765000
C	5.634153000	-0.239017000	-2.463282000
H	6.207585000	-0.803273000	-3.215308000
H	4.730696000	0.146230000	-2.957041000
H	6.248983000	0.618233000	-2.157400000
C	4.403564000	-2.953035000	-1.771902000
H	3.371197000	-2.750793000	-2.088520000
H	4.973933000	-3.279358000	-2.655492000
H	4.372048000	-3.795636000	-1.068486000
C	3.358832000	-2.834546000	1.487645000
H	2.690271000	-3.298403000	0.749336000
H	4.363749000	-3.263909000	1.371511000
H	2.999505000	-3.108325000	2.487582000
C	1.944586000	-0.672564000	3.415956000
H	1.646152000	-1.724816000	3.478264000
H	2.540602000	-0.441583000	4.314054000
H	1.035399000	-0.059657000	3.449567000

C	2.624660000	2.190648000	2.404234000
H	1.541843000	2.178938000	2.586991000
H	3.126908000	2.298297000	3.379135000
H	2.859537000	3.083305000	1.812629000
C	4.537612000	1.956585000	-0.176236000
H	5.624398000	1.994478000	-0.001522000
H	4.375154000	1.873583000	-1.256926000
H	4.117984000	2.915161000	0.151514000
C	0.123783000	5.403820000	1.940933000
H	0.443016000	6.152802000	1.203470000
H	-0.141227000	5.944446000	2.863068000
H	0.985089000	4.764655000	2.175650000
C	-2.816781000	5.684367000	1.191194000
H	-3.775037000	5.212751000	0.934048000
H	-2.962279000	6.235221000	2.133071000
H	-2.588336000	6.421587000	0.407440000
C	-1.835163000	3.193482000	2.763443000
H	-1.118789000	2.360543000	2.785842000
H	-1.807315000	3.700390000	3.740450000
H	-2.839590000	2.762953000	2.647150000
C	1.261420000	4.355092000	-1.015613000
H	1.155139000	5.427873000	-1.244651000
H	1.616998000	4.266436000	0.014448000
H	2.038172000	3.948528000	-1.673747000
C	0.439438000	2.915748000	-3.690323000
H	0.441735000	3.857485000	-4.261731000
H	1.480426000	2.688650000	-3.424019000
H	0.086877000	2.124660000	-4.364363000
C	-2.618267000	1.930334000	-3.420090000
H	-3.218895000	2.691183000	-3.943844000
H	-1.997405000	1.429590000	-4.174070000
H	-3.311740000	1.186266000	-3.009171000
C	-3.648303000	2.679674000	-0.535606000
H	-3.705870000	2.623176000	0.556614000
H	-4.289116000	3.514553000	-0.861900000
H	-4.078565000	1.756692000	-0.942238000
C	-5.669719000	-1.199593000	-0.842951000
H	-6.451218000	-1.419574000	-1.587185000
H	-6.160045000	-1.134897000	0.137750000
H	-5.262268000	-0.208176000	-1.084341000
C	-3.679717000	-2.555867000	-2.707966000
H	-3.069735000	-3.438888000	-2.941509000
H	-4.510834000	-2.529313000	-3.430153000
H	-3.053472000	-1.667938000	-2.873100000
C	-5.304550000	-4.214453000	-0.660683000
H	-6.122215000	-4.314567000	-1.391142000
H	-4.657968000	-5.096475000	-0.766164000
H	-5.750409000	-4.250062000	0.344396000
C	-3.864749000	-0.368178000	1.816199000
H	-4.145619000	0.172825000	0.908461000
H	-4.793460000	-0.707843000	2.303911000
H	-3.382319000	0.343592000	2.497559000
C	-1.638876000	-1.372390000	3.769035000
H	-1.582413000	-0.276358000	3.736758000
H	-2.436685000	-1.640896000	4.480186000
H	-0.694776000	-1.742323000	4.184045000
C	-0.289103000	-4.041388000	2.493683000
H	0.461635000	-4.371587000	1.764270000
H	0.238669000	-3.524896000	3.304732000
H	-0.752253000	-4.942021000	2.928861000
C	-1.806227000	-4.730329000	-0.141655000
H	-2.370070000	-5.556207000	0.322652000
H	-2.141982000	-4.643573000	-1.180996000
H	-0.749226000	-5.027356000	-0.150429000
K'			
Ti	-0.569590000	1.327320000	-0.546048000

H	-1.495394000	-0.198508000	-1.081648000
Ti	1.760040000	-0.280857000	0.116937000
Ti	-0.833133000	-1.494011000	0.231293000
Si	-1.318328000	4.701144000	1.135815000
Si	5.212118000	-1.101048000	-1.184549000
Si	-4.430511000	-2.425950000	-0.901992000
N	1.010267000	-1.903373000	-0.366967000
N	-0.120373000	0.269007000	0.823051000
C	0.139081000	-2.565035000	-2.567553000
H	-0.540231000	-3.288865000	-3.038705000
C	0.315020000	-2.864876000	-1.072609000
C	0.704539000	-4.317123000	-0.799323000
H	-0.015266000	-5.022792000	-1.233466000
H	0.797756000	-4.516532000	0.275027000
H	1.687665000	-4.526033000	-1.257702000
C	-1.149026000	3.621211000	-0.421702000
C	-2.261786000	2.943689000	-1.057074000
C	-1.833216000	2.428668000	-2.323300000
C	-0.456016000	2.783679000	-2.497109000
C	-0.036405000	3.517243000	-1.341705000
C	4.144768000	-0.440007000	0.236388000
C	3.571225000	-1.225077000	1.295822000
C	2.878582000	-0.349588000	2.195538000
C	3.057816000	0.995257000	1.730026000
C	3.822981000	0.944301000	0.529413000
C	-3.112721000	-2.257691000	0.458398000
C	-2.246473000	-3.345899000	0.854657000
C	-1.500984000	-2.940196000	2.010968000
C	-1.932865000	-1.617443000	2.370260000
C	-2.915589000	-1.203594000	1.429660000
H	1.113189000	-2.616961000	-3.086468000
H	1.117563000	1.111654000	-1.059011000
H	-0.254474000	-1.551140000	-2.728369000
H	2.354774000	-0.223642000	-1.504380000
C	6.947162000	-1.470792000	-0.481109000
H	6.902771000	-2.213220000	0.329699000
H	7.615578000	-1.869783000	-1.259604000
H	7.417764000	-0.564762000	-0.070866000
C	5.413730000	0.133942000	-2.616622000
H	5.972412000	-0.360167000	-3.427045000
H	4.437022000	0.435006000	-3.020369000
H	5.969919000	1.039435000	-2.339596000
C	4.523532000	-2.699384000	-1.955153000
H	3.439096000	-2.615878000	-2.104056000
H	4.991679000	-2.858335000	-2.939282000
H	4.723498000	-3.596784000	-1.352937000
C	3.723830000	-2.712319000	1.511831000
H	3.834926000	-3.251542000	0.566438000
H	4.611951000	-2.923959000	2.129991000
H	2.853100000	-3.133455000	2.030546000
C	4.295362000	2.143783000	-0.256777000
H	5.392457000	2.225697000	-0.216188000
H	4.006235000	2.081016000	-1.312078000
H	3.885013000	3.074581000	0.151848000
C	2.555897000	2.216240000	2.458494000
H	3.118746000	2.374156000	3.392603000
H	2.666788000	3.123672000	1.852963000
H	1.494543000	2.115842000	2.724079000
C	2.255517000	-0.725889000	3.515505000
H	1.415375000	-0.067481000	3.765544000
H	1.887634000	-1.759184000	3.511470000
H	2.995190000	-0.647048000	4.329908000
C	-0.598158000	-3.822015000	2.840878000
H	-1.183141000	-4.349933000	3.611795000
H	-0.094867000	-4.584046000	2.234608000
H	0.175877000	-3.242459000	3.358026000
C	-2.309779000	-4.762127000	0.337397000

H	-3.138614000	-5.298327000	0.826561000
H	-2.478119000	-4.806387000	-0.745236000
H	-1.392457000	-5.317645000	0.557013000
C	-1.518482000	-0.822703000	3.581844000
H	-2.359626000	-0.737909000	4.288314000
H	-0.687719000	-1.300194000	4.112940000
H	-1.205362000	0.191562000	3.302313000
C	-3.614275000	0.125594000	1.527636000
H	-4.138149000	0.381954000	0.605428000
H	-4.354857000	0.117425000	2.344768000
H	-2.894020000	0.925496000	1.750220000
C	-5.561324000	-0.906822000	-1.083210000
H	-6.092884000	-0.652799000	-0.155756000
H	-5.025171000	-0.012373000	-1.428339000
H	-6.323477000	-1.139831000	-1.843295000
C	-5.588353000	-3.871508000	-0.454104000
H	-6.420151000	-3.919786000	-1.173721000
H	-5.083967000	-4.846607000	-0.469402000
H	-6.023890000	-3.737080000	0.547001000
C	-3.660875000	-2.746050000	-2.609393000
H	-3.050481000	-3.658888000	-2.636500000
H	-4.453126000	-2.855076000	-3.366311000
H	-3.016071000	-1.909816000	-2.913960000
C	-1.840658000	3.694310000	2.662639000
H	-1.841467000	4.339619000	3.554837000
H	-2.848808000	3.266569000	2.569567000
H	-1.143597000	2.864552000	2.847381000
C	0.279207000	5.622394000	1.593985000
H	0.660216000	6.248112000	0.775556000
H	0.055131000	6.290550000	2.440269000
H	1.086295000	4.951270000	1.916455000
C	-2.629655000	6.038502000	0.790826000
H	-3.628792000	5.619695000	0.609590000
H	-2.709333000	6.721315000	1.650584000
H	-2.357848000	6.641891000	-0.087755000
C	1.329220000	4.144182000	-1.207513000
H	1.310849000	5.187529000	-1.562465000
H	1.680032000	4.154127000	-0.171643000
H	2.068581000	3.602391000	-1.807828000
C	-3.698154000	2.960189000	-0.590693000
H	-3.781479000	3.018124000	0.500343000
H	-4.217846000	3.836762000	-1.009655000
H	-4.248590000	2.072282000	-0.923417000
C	-2.701626000	1.739232000	-3.348336000
H	-3.545138000	1.217555000	-2.881538000
H	-3.117144000	2.471147000	-4.059525000
H	-2.135982000	1.000571000	-3.930437000
C	0.396477000	2.471540000	-3.702987000
H	0.479133000	3.350352000	-4.362296000
H	1.410604000	2.170123000	-3.412238000
H	-0.033129000	1.654849000	-4.296360000

TS12'

Ti	1.230499000	-1.103227000	0.646093000
H	-0.515706000	-1.705874000	1.256440000
Ti	0.477550000	1.276408000	-0.076418000
Ti	-1.571634000	-0.730831000	0.132733000
Si	3.597513000	-2.703714000	-1.799027000
Si	2.033541000	4.720527000	0.546581000
Si	-5.327060000	0.366577000	-0.236346000
N	-1.262587000	0.862403000	1.028439000
N	0.059124000	-0.599683000	-0.788057000
C	0.872332000	0.720751000	2.094966000
H	0.743043000	-0.471957000	2.313819000
C	-0.600039000	1.228391000	2.286058000
C	-1.284252000	0.623480000	3.525628000
H	-1.301814000	-0.471445000	3.447248000

H	-2.317923000	0.987328000	3.593335000
H	-0.747725000	0.910615000	4.442661000
C	3.082973000	-2.355227000	-0.005624000
C	2.213288000	-3.216901000	0.771637000
C	2.186931000	-2.762921000	2.127093000
C	3.091667000	-1.647840000	2.225989000
C	3.630857000	-1.390523000	0.937813000
C	1.071785000	3.516851000	-0.552704000
C	-0.365767000	3.418873000	-0.680007000
C	-0.676115000	2.553730000	-1.772078000
C	0.552944000	2.097882000	-2.344850000
C	1.626090000	2.689136000	-1.607161000
C	-3.961394000	-0.952525000	-0.244405000
C	-3.283830000	-1.585299000	-1.363113000
C	-2.585524000	-2.736891000	-0.892358000
C	-2.784843000	-2.824246000	0.523234000
C	-3.630341000	-1.736942000	0.919188000
H	1.542288000	0.987470000	2.927774000
H	2.100789000	0.403454000	-0.075763000
H	-0.574657000	2.324670000	2.424691000
H	1.459891000	1.702787000	1.334564000
C	4.683495000	-0.346575000	0.653284000
H	5.690105000	-0.794081000	0.685093000
H	4.546654000	0.111833000	-0.329516000
H	4.658543000	0.456881000	1.400130000
C	3.446521000	-0.945671000	3.512615000
H	4.224812000	-1.504322000	4.056727000
H	3.833790000	0.065657000	3.336425000
H	2.579894000	-0.864504000	4.184178000
C	1.483923000	-3.431520000	3.283686000
H	2.131875000	-4.192689000	3.749143000
H	1.213459000	-2.708235000	4.063918000
H	0.562848000	-3.932326000	2.962327000
C	1.527626000	-4.468314000	0.278052000
H	1.264715000	-4.403109000	-0.783169000
H	2.193706000	-5.337408000	0.402847000
H	0.612171000	-4.677700000	0.843836000
C	4.766494000	-1.387791000	-2.516853000
H	5.706617000	-1.294953000	-1.956423000
H	5.025326000	-1.683579000	-3.545670000
H	4.300340000	-0.394685000	-2.568825000
C	4.543537000	-4.358887000	-1.826943000
H	3.923493000	-5.197210000	-1.478436000
H	4.877650000	-4.598226000	-2.848265000
H	5.436146000	-4.318594000	-1.185240000
C	2.107314000	-2.820332000	-2.974659000
H	1.546165000	-3.759022000	-2.862396000
H	1.409685000	-1.989528000	-2.800590000
H	2.453091000	-2.773229000	-4.019294000
C	3.090582000	2.571787000	-1.961223000
H	3.458791000	3.510801000	-2.405583000
H	3.709636000	2.348565000	-1.086209000
H	3.256008000	1.777495000	-2.698581000
C	0.661256000	1.188678000	-3.543529000
H	0.388485000	1.723528000	-4.467326000
H	1.680832000	0.806884000	-3.669772000
H	-0.001546000	0.320406000	-3.438994000
C	-2.058257000	2.201215000	-2.249171000
H	-2.638219000	3.103260000	-2.498000000
H	-2.014205000	1.574399000	-3.146886000
H	-2.624780000	1.652607000	-1.478812000
C	-1.407779000	4.157212000	0.128210000
H	-1.262942000	4.047636000	1.209911000
H	-1.384691000	5.235462000	-0.097604000
H	-2.412631000	3.789141000	-0.107324000
C	3.772250000	4.092505000	1.000833000
H	3.747714000	3.055418000	1.364730000

H	4.474913000	4.138992000	0.157985000
H	4.183871000	4.720650000	1.806130000
C	2.221435000	6.364542000	-0.398596000
H	1.241558000	6.801062000	-0.642328000
H	2.778064000	7.105425000	0.195467000
H	2.762348000	6.223456000	-1.345997000
C	1.149103000	5.093471000	2.191204000
H	0.213738000	5.653481000	2.059253000
H	0.919716000	4.177873000	2.755943000
H	1.812344000	5.708086000	2.819758000
C	-2.368149000	-3.958557000	1.426976000
H	-2.054454000	-3.599018000	2.415350000
H	-3.207491000	-4.656620000	1.578859000
H	-1.538124000	-4.532724000	1.000098000
C	-4.159742000	-1.552628000	2.323161000
H	-4.437271000	-0.511294000	2.522712000
H	-5.053582000	-2.175581000	2.491166000
H	-3.417209000	-1.847888000	3.076543000
C	-1.821382000	-3.703349000	-1.763187000
H	-1.236556000	-4.408661000	-1.161131000
H	-2.507163000	-4.295610000	-2.390109000
H	-1.125069000	-3.182956000	-2.434606000
C	-3.377532000	-1.224795000	-2.828115000
H	-4.172859000	-1.809272000	-3.319830000
H	-3.605217000	-0.166755000	-2.982621000
H	-2.438651000	-1.450170000	-3.351664000
C	-4.935908000	1.816826000	0.933083000
H	-5.116129000	1.558842000	1.986874000
H	-3.884003000	2.120204000	0.846566000
H	-5.572888000	2.683104000	0.696357000
C	-5.716862000	1.082478000	-1.956691000
H	-5.989580000	0.302003000	-2.680672000
H	-6.586345000	1.751080000	-1.855156000
H	-4.900324000	1.676470000	-2.387970000
C	-6.935447000	-0.476713000	0.342652000
H	-7.767945000	0.243856000	0.341347000
H	-7.211526000	-1.305266000	-0.326126000
H	-6.854126000	-0.884769000	1.359523000

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