Supporting Information

Aluminacyclopropene-Phosphine Complex: A Carbene-Exchange Reagent

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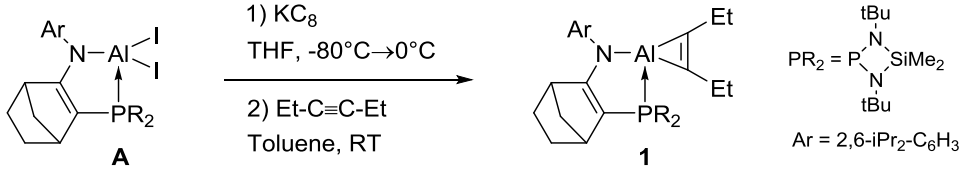
Contents

1-General

All manipulations were performed under inert atmosphere of argon by using Schlenk or high-pressure NMR tube techniques. Dry, oxygen-free solvents were employed. The melting point analysis were carried out in a Stuart SMP40 machine. ^{1}H, ^{13}C, ^{29}Si and ^{31}P NMR spectra were recorded on Bruker Avance NEO 300 MHz, Avance II 400 MHz, Avance III HD 400 MHz, Avance III HD 500 MHz and Avance NEO 600 MHz spectrometers ^{1}H and ^{13}C NMR chemical shifts are reported in ppm relative tetramethylsilane (δ = 0 ppm) and were calibrated against the residual proton and natural abundance carbon resonances of the respective deuterated solvent as internal standard. ^{29}Si NMR chemical shifts were referenced to the signal of tetramethylsilane (δ = 0 ppm) as external standard. ^{31}P NMR chemical shifts are expressed in ppm relative to 85 % H_3PO_4. The following abbreviations and their combinations are used: br, broad; s, singlet; d, doublet; t, triplet; q, quartet; sept, septuplet m, multiplet. ^{1}H and ^{13}C resonance signals were attributed by means of 2D COSY, HSQC and HMBC experiments. ESI-HRMS data were obtained on a Waters Xevo G2 Q-TOF mass spectrometer. The phosphine-stabilized diiodoalane complex **A** was synthesized as previously reported (S1).

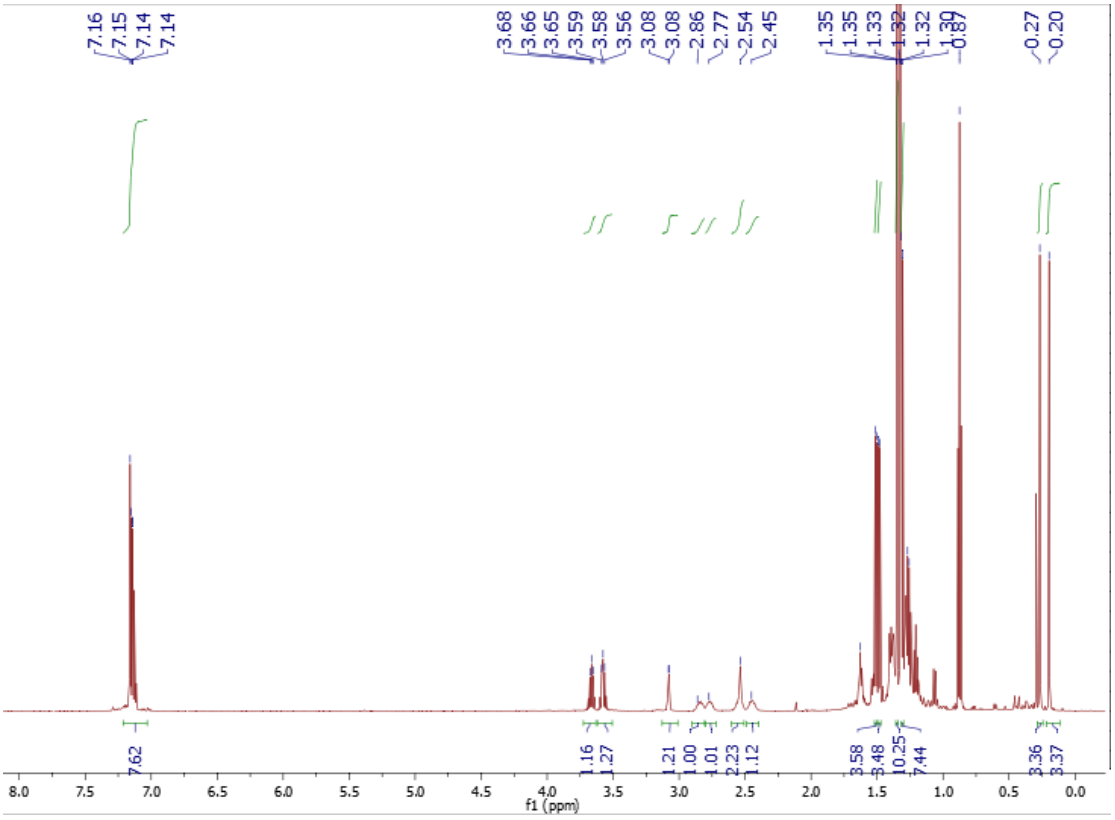
2-Experimental procedures and characterization data



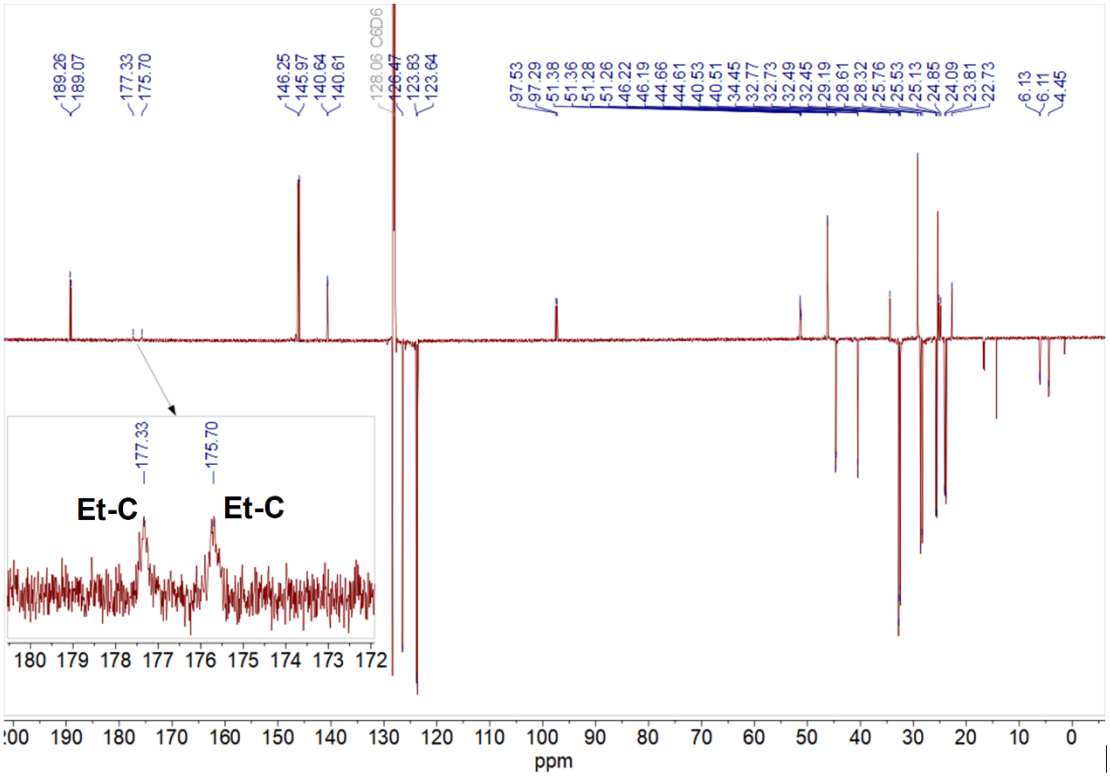
Synthesis of 1: To a mixture of diiodoalane **A** (200 mg, 0.26 mmol) and KC_8 (86 mg, 0.64 mmol, 2.5 eqv.), THF (10 ml) was added at –80 °C. After stirring for 1 hr at –80 °C, all volatiles were removed under vacuum at 0 °C. The resulting solid was washed with pentane (2 x 2ml), and then the crude product was extracted with the solution of toluene (10 ml) containing 3-Hexyne (0.06 ml, 0.52 mmol) at rt. After that, left crude product was extracted with toluene (3ml X 3). Then, all combined solution was concentrated to 3 ml and kept at –25 °C overnight to obtain **1** as yellow crystals (117 mg, yield = 75 %). Mp: 163-168 °C (decomp.).

^{1}H NMR (600 MHz, C_6D_6, 25 °C): δ 0.20 (s, 3H, $SiCH_3$), 0.27 (s, 3H, $SiCH_3$), 1.06 (m, 1H, CH_2), 1.27 (m, 6H, CH_{3Et}), 1.31 (d, J_{HH} = 6.9 Hz, 6H, CH_{3iPr}), 1.32 (s, 9H, CH_{3tBu}), 1.35 (s, 9H, CH_{3tBu}), 1.37 (m, 2H, CH_2), 1.38 (m, 6H, CH_{3Et}), 1.48 (d, J_{HH} = 6.8 Hz, 3H, CH_{3iPr}), 1.51 (d, J_{HH} = 7.0 Hz, 3H, CH_{3iPr}), 1.54 (m, 1H, CH_2), 1.60 (m, 2H, CH_2), 2.45 (dq, J_{HH} = 7.4 Hz, $J_{HH(gem)}$ = 14.2 Hz, 1H, CH_{2Et}), 2.54 (superposed, 1H, CH_{2Et}), 2.54 (s, 1H, $CH_{bridgehead}$), 2.77 (dq, J_{HH} = 6.8 Hz, $J_{HH(gem)}$ = 13.5 Hz, 1H, CH_{2Et}), 2.84 (dq, J_{HH} = 6.8 Hz, $J_{HH(gem)}$ = 13.7 Hz, 1H, CH_{2Et}), 3.08 (s, 1H, $CH_{bridgehead}$), 3.58 (sept, J_{HH} = 7.0 Hz, 1H, CH_{iPr}), 3.66 (sept, J_{HH} = 7.0 Hz, 1H, CH_{iPr}), 7.14 (m, 3H, CH_{Ar}).
^{13}C{^{1}H} NMR (151 MHz, C_6D_6, 25 °C): δ 4.5 (d, J_{CP} = 1.5 Hz, $SiCH_3$), 6.1 (d, J_{CP} = 3.0 Hz, $SiCH_3$), 16.6 (br, CH_{3Et}), 16.8 (br, CH_{3Et}), 23.8 (s, CH_{3iPr}), 24.1 (s, CH_{3iPr}), 24.9 (br, CH_{2Et}),25.3 (br, CH_{2Et}), 25.4 (d, J_{CP} = 1.0 Hz, CH_2), 25.5 (s, CH_{3iPr}), 25.8 (s, CH_{3iPr}), 28.3 (s, CH_{iPr}), 28.6 (s, CH_{iPr}), 29.1 (s, CH_2), 32.5 (d, J_{CP} = 6.3 Hz, CH_{3tBu}), 32.8 (d, J_{CP} = 5.8 Hz, CH_{3tBu}), 40.5 (d, J_{CP} = 3.6 Hz, $CH_{bridgehead}$), 44.6 (d, J_{CP} = 8.1 Hz, $CH_{bridgehead}$), 46.2 (d, J_{CP} = 5.3 Hz, CH_2), 51.3 (d, J_{CP} = 2.3 Hz, C_{tBu}), 51.4 (d, J_{CP} = 3.3 Hz, C_{tBu}), 97.4 (d, J_{CP} = 37.2 Hz CP), 123.6 (s, CH_{Ar}), 123.8 (s, CH_{Ar}), 126.5 (s, CH_{Ar}), 140.6 (d, J_{CP} = 3.8 Hz, N-C_{Ar}), 146.0 (s, iPr-C_{Ar}), 146.3 (s, iPr-C_{Ar}), 175.7 (br, Al-C), 177.3 (br, Al-C), 189.1 (d, J_{CP} = 29.5 Hz, CN).
^{31}P{^{1}H} NMR (243 MHz, C_6D_6, 25 °C): δ 54.9 (s, PN).
^{29}Si{^{1}H} NMR (99 MHz, C_6D_6, 25 °C): δ 11.0 (d, J_{SiP} = 3.7 Hz, $SiCH_3$).

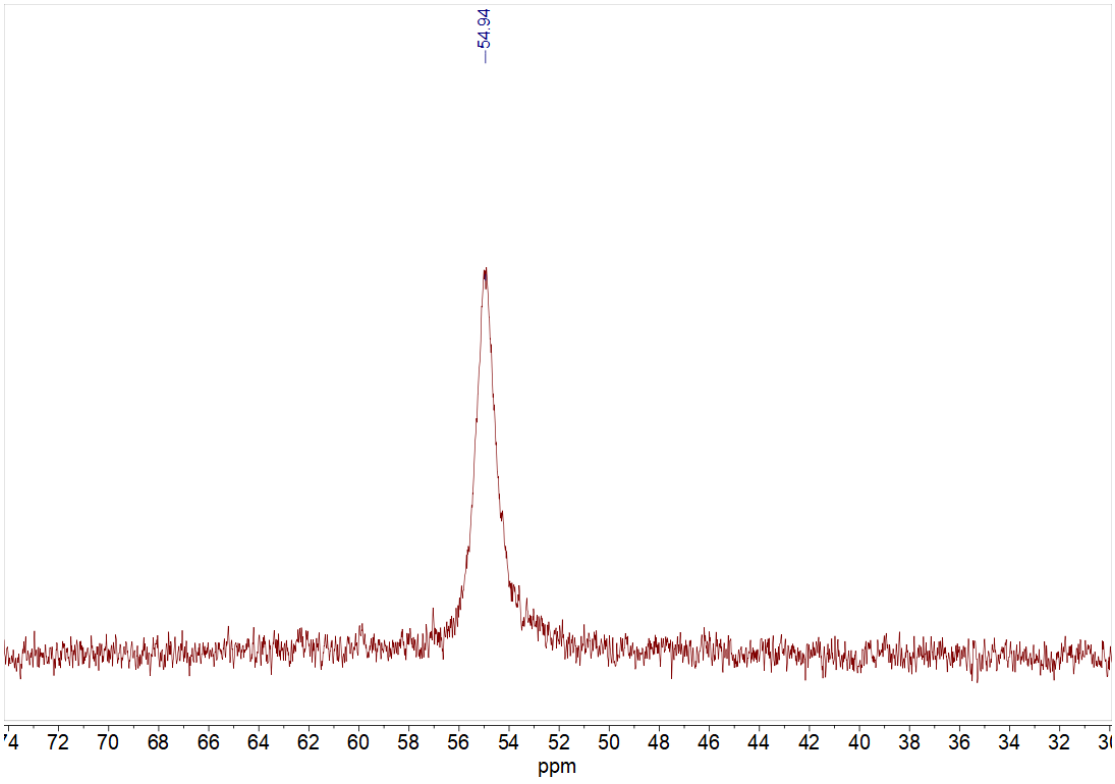
^{1}H NMR (600 MHz, C_6D_6, 25 ^{o}C):



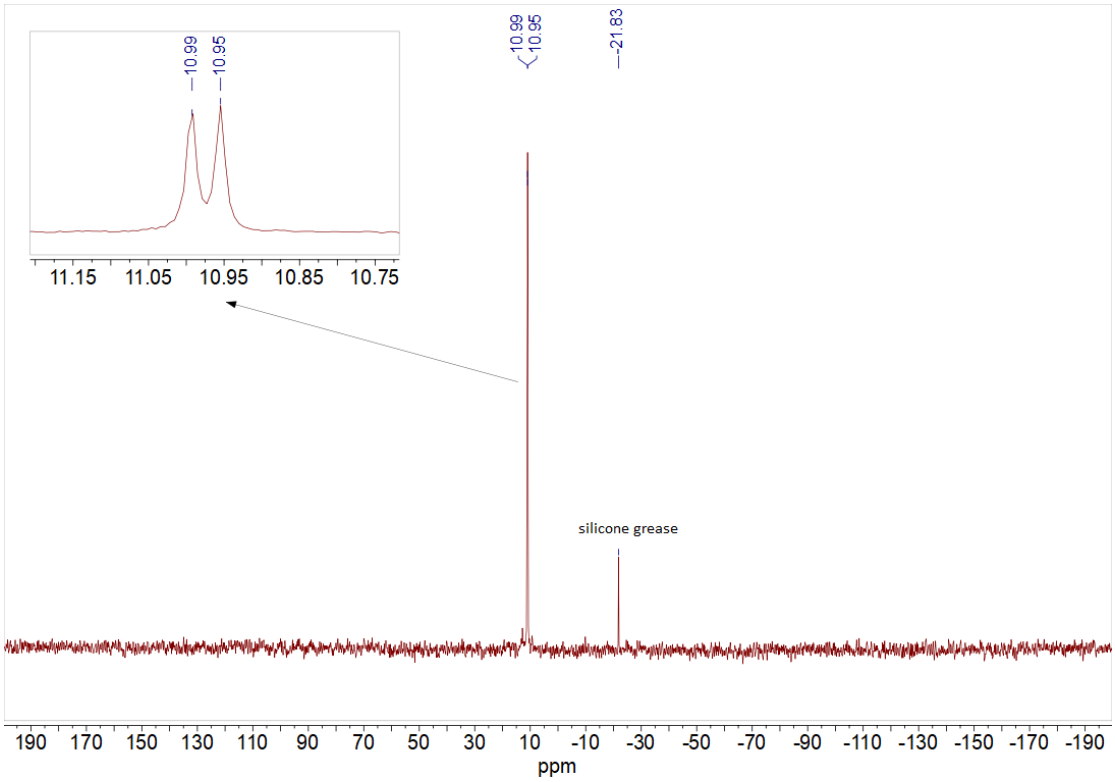
^{13}C{^{1}H} NMR (151 MHz, C_6D_6, 25 ^{o}C):

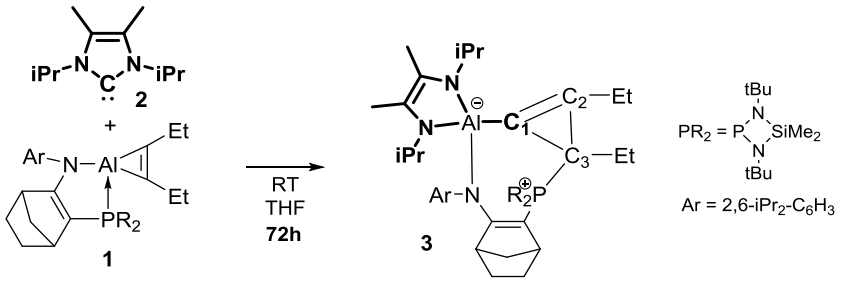


$^{31}P\{^{1}H\}$ NMR (243 MHz, C_6D_6, 25 °C):



$^{29}Si\{^{1}H\}$ NMR (99 MHz, C_6D_6, 25 °C):





Synthesis of 3: To a solution of **1** (0.2 g, 0.329 mmol) in toluene (5 ml), NHC (0.06 g, 0.329 mmol) in toluene (2.5 ml) was added at room temperature. After stirring for 72 hours, the solution was filtrated and dried under vacuum. The crude product was extracted by pentane (2 X 5 ml). The solution was concentrated to 2.5 ml and store at –25 °C to obtain **3** as pale brown crystals (0.15 g, yield = 58 %). Mp: 178-188 °C (decomp.).

^{1}H NMR (500 MHz, Toluene-d_8, 25 °C): δ 0.28 (s, 3H, $SiCH_3$), 0.31 (s, 3H, $SiCH_3$), 0.90 (t, J_{HH} = 7.5 Hz, 3H, CH_{3Et}), 0.92 (s, 1H, CH_2), 1.09 (s, 9H, CH_{3tBu}), 1.11 (d, J_{HH} = 6.7 Hz, 3H, CH_{3iPr}), 1.14 (d, J_{HH} = 6.6 Hz, 3H, CH_{3iPr}), 1.16 (d, J_{HH} = 6.5 Hz, 3H, CH_{3NiPr}), 1.27 (m, 3H, CH_{3Et}), 1.28 ($d_{overlapped}$, 6H, CH_{3NiPr}), 1.30 (s, 9H, CH_{3tBu}), 1.42 (s, 1H, CH_2), 1.50 (d, J_{HH} = 6.6 Hz, 3H, CH_{3NiPr}), 1.52 (s, 2H, CH_2), 1.59 (m, 6H, CH_{3iPr}), 1.62 (m, 2H, CH_2), 1.78 (d, J_{cp} = 1.0 Hz, 3H, CH_3), 1.80 (d, J_{cp} = 1.0 Hz, 3H, CH_3), 1.85 (m, 1H, CH_{2Et}), 2.34 (m, 1H, CH_{2Et}), 2.64 (m, 1H, CH_{2Et}), 2.87 (m, 1H, $CH_{bridgehead}$), 2.89 (m, 1H, CH_{2Et}), 3.21(m, 1H, $CH_{bridgehead}$), 3.37 (sept, J_{HH} = 6.6 Hz, 1H, CH_{iPr}), 3.48 (sept, J_{HH} = 6.8 Hz, 1H, CH_{NiPr}), 3.49 (sept, J_{HH} = 6.8 Hz, 1H, CH_{iPr}), 3.72 (sept, J_{HH} = 6.3 Hz, 1H, CH_{NiPr}), 7.11 – 7.18 (m, 3H, CH_{Ar}).

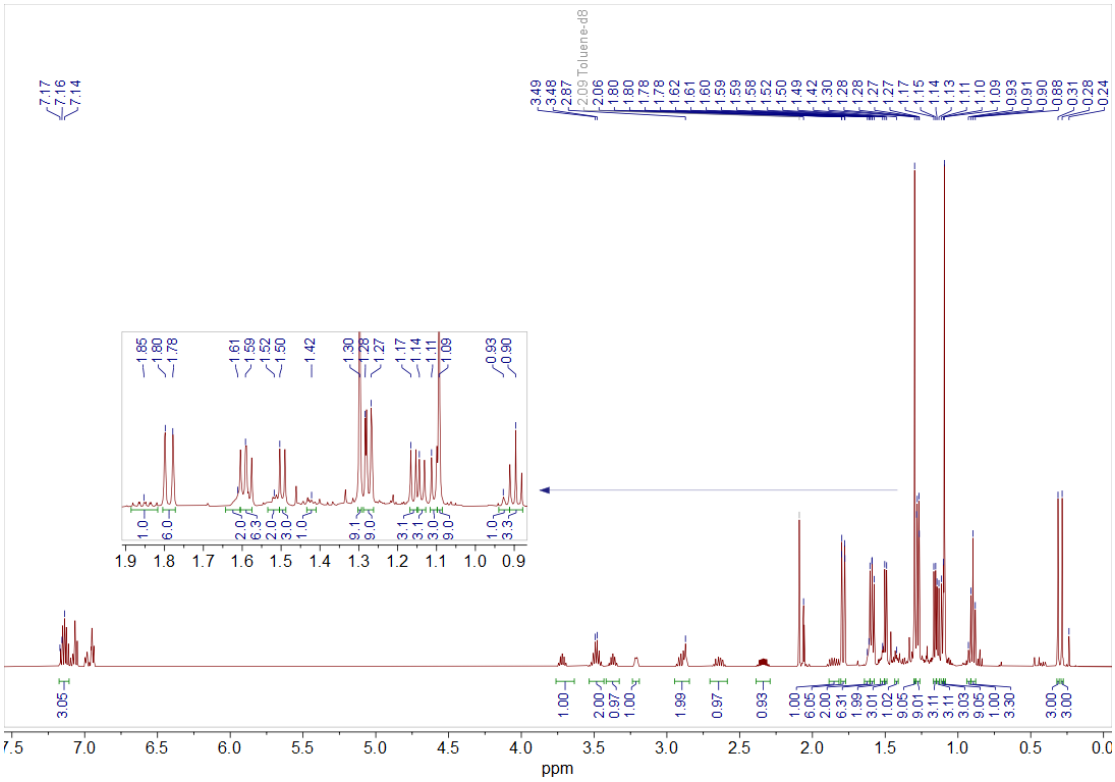
^{13}C{^{1}H} NMR (126 MHz, Toluene-d_8, 25 °C): δ 5.3 (d, J_{cp} = 1.7 Hz, $SiCH_3$), 5.8 (s, $SiCH_3$), 12.7 (d, J_{cp} = 4.7 Hz, CH_{3Et}), 13.9 (s, CH_3), 14.6 (d, J_{cp} = 2.9 Hz, CH_{3Et}), 17.0 (s, CH_3), 22.70 (d, J_{cp} = 2.7 Hz, CH_{2Et}), 25.3 (s, CH_{3iPr} x 2), 26.2 (s, CH_{3NiPr} x 2), 27.1 (d, J_{cp} = 108.0 Hz, Et-C_3-P), 27.4 (s, CH_{3NiPr} x 2), 27.5 (s, CH_{3iPr}), 28.0 (d, J_{cp} = 2.1 Hz, CH_{2Et}), 28.3 (s, CH_{3iPr}), 28.4 (s, CH_{iPr}), 29.1 (d, J_{cp} = 32.4 Hz, CH_2), 29.6 (s, CH_{iPr}), 30.2 (s, CH_2), 33.3 (d, J_{cp} = 4.6 Hz, CH_{3tBu}), 33.6 (d, J_{cp} = 4.1 Hz, CH_{3tBu}), 44.7 (d, J_{cp} = 4.5 Hz, CH_2), 46.3 (d, J_{cp} = 12.7 Hz, $CH_{bridgehead}$), 47.0 (s, CH_{NiPr}), 47.9 (s, CH_{NiPr}), 50.7 (d, J_{cp} = 12.5 Hz, $CH_{bridgehead}$), 52.4 (s, C_{tBu}), 52.8 (s, C_{tBu}), 82.0 (d, J_{cp} = 116.8 Hz, PC), 119.7 (br, detected by HMQC (^{31}P, ^{13}C) experiment, Al-C_1), 121.2 (s, Me-C=C), 123.9 (s, CH_{Ar}), 124.4 (s, Me-C=C), 124.5 (s, CH_{Ar}), 126.3 (s, CH_{Ar}), 130.8 (s, Et-C_2), 143.9 (s, N-C_{Ar}), 146.3 (s, iPr-C_{Ar}), 146.5 (s, iPr-C_{Ar}), 180.7 (d, J_{cp} = 9.5 Hz, NC).

^{31}P{^{1}H} NMR (121 MHz, Toluene-d_8, 25 °C) δ 68.5 (CP).

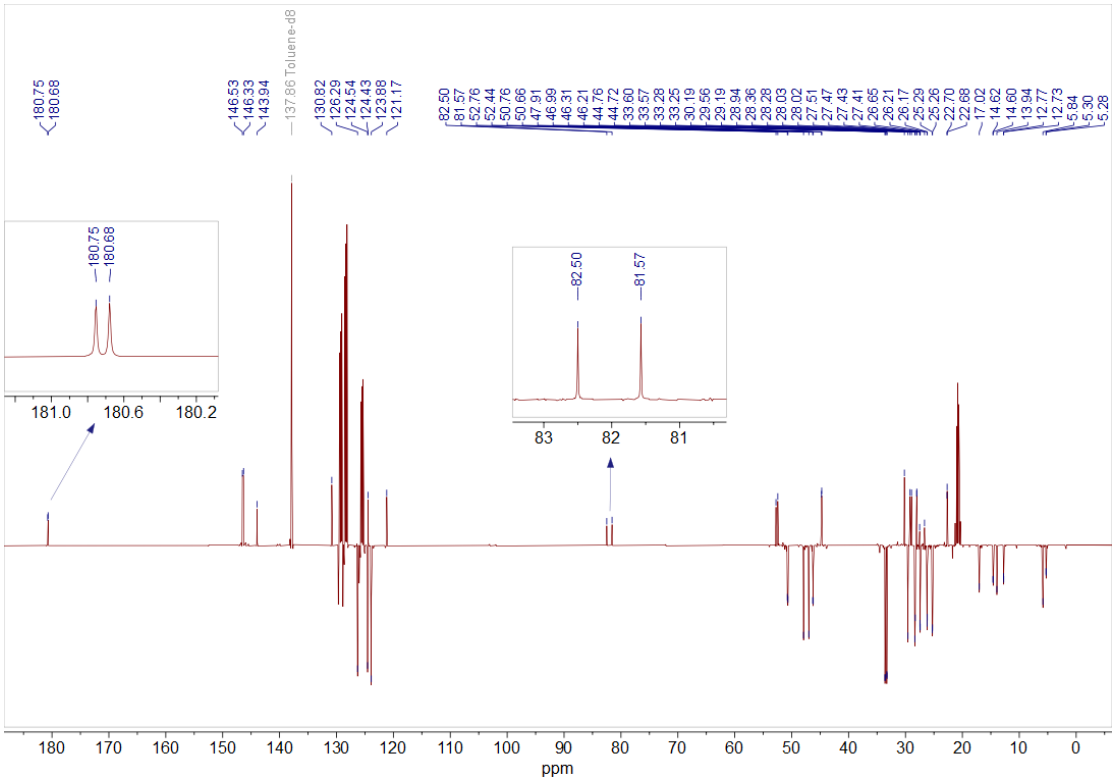
^{29}Si{^{1}H} NMR (99 MHz, Toluene-d_8, 25 °C) δ 9.6 ($SiCH_3$).

HRMS (ESI): m/z $[M]^+$ calcd for $C_{46}H_{80}AlN_5PSi$: 788.5736; found: 788.5757

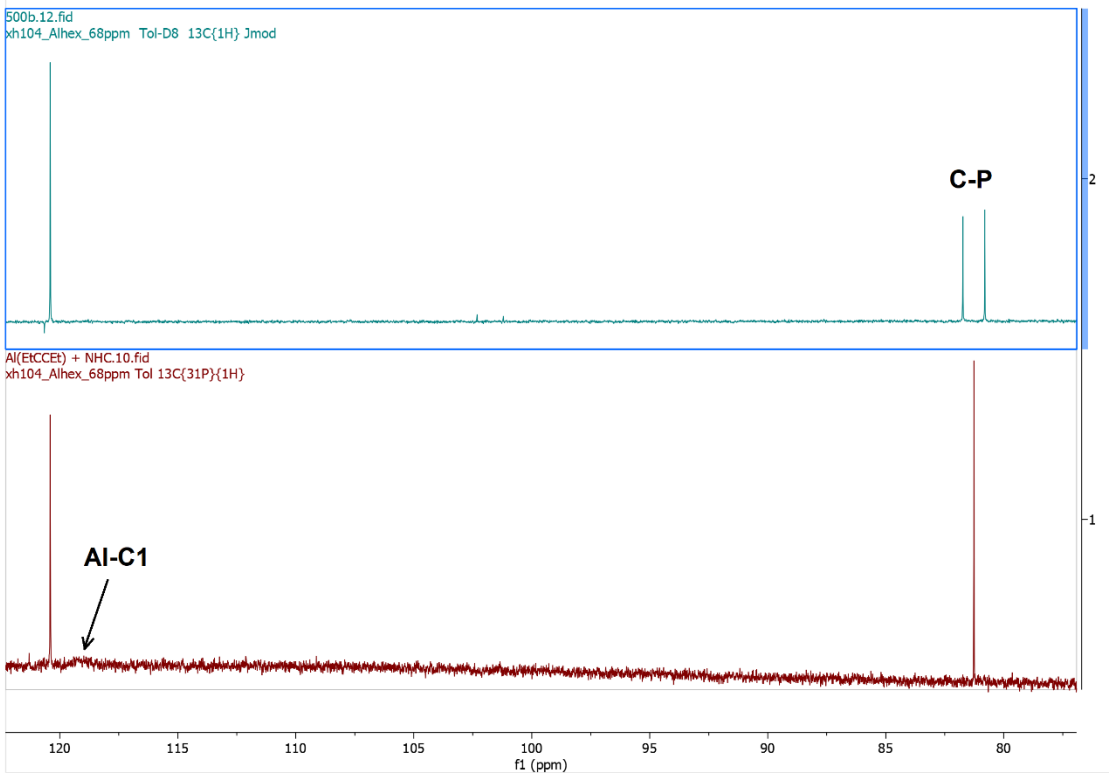
^{1}H NMR (500 MHz, Toluene-d_8, 25 ^{o}C):



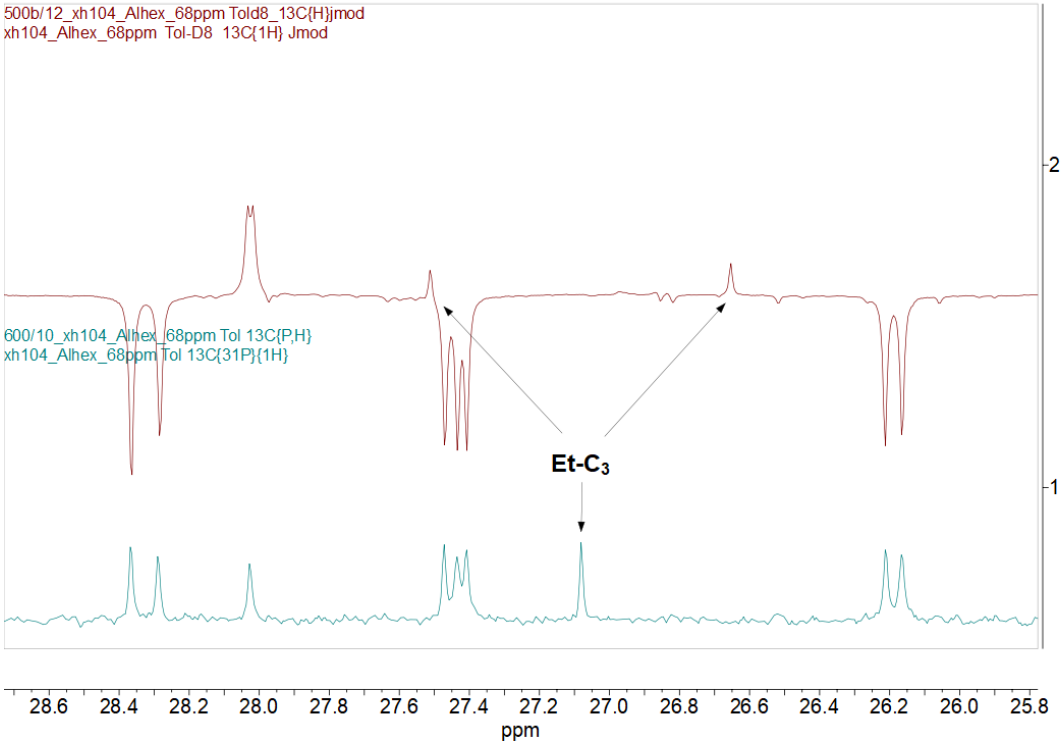
^{13}C{^{1}H} NMR (126 MHz, Toluene-d_8, 25 ^{o}C):



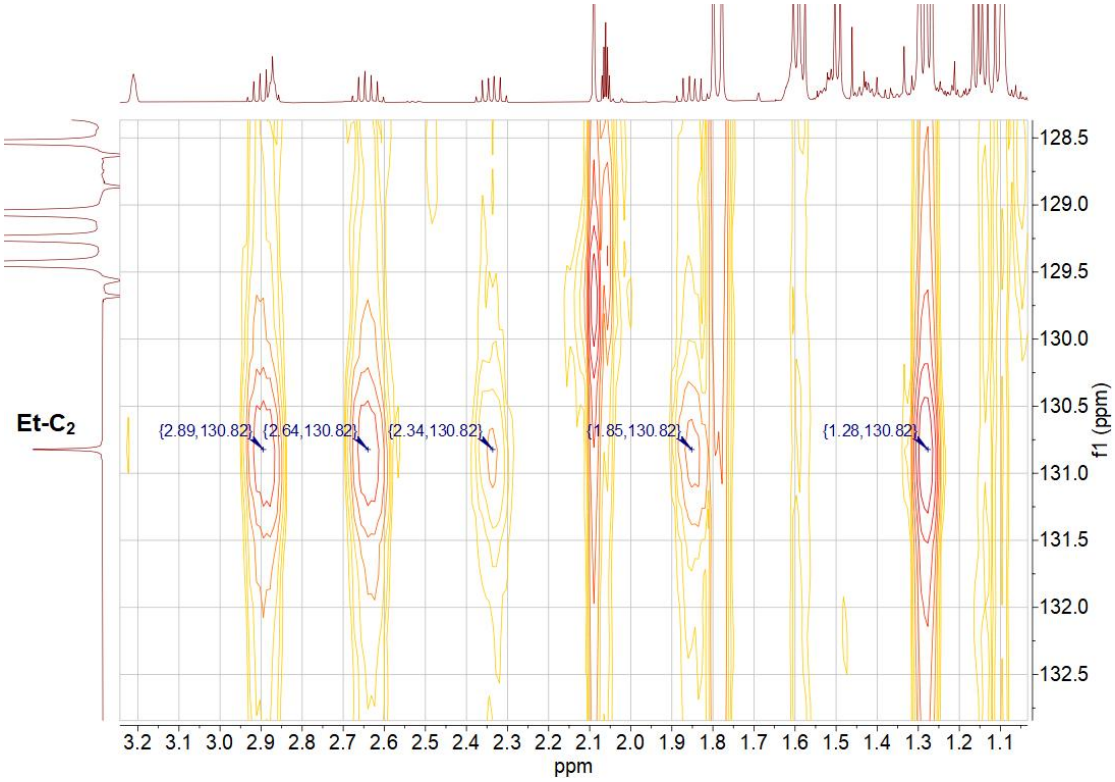
$^{13}C\{^{1}H\}$-NMR (upside) and $^{13}C\{^{1}H,^{31}P\}$-NMR (downside) (126 MHz, Toluene-d_8, 25 °C):



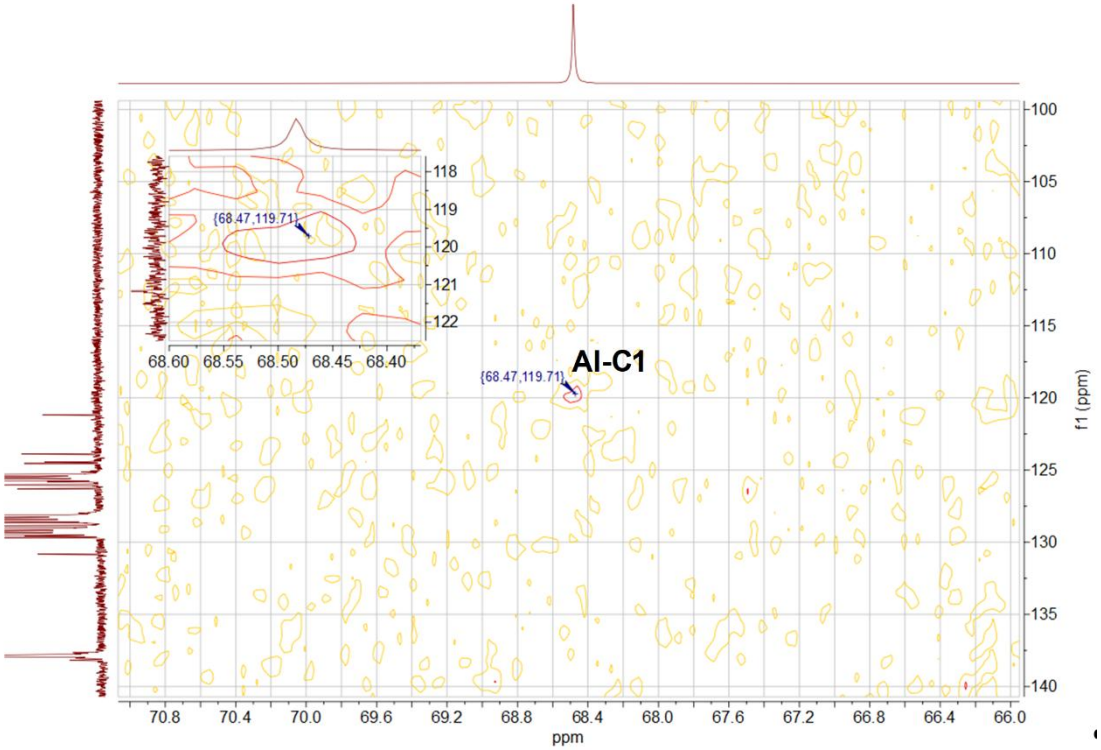
$^{13}C\{^{1}H\}$-NMR (upside) and $^{13}C\{^{1}H,^{31}P\}$-NMR (downside) (126 MHz, Toluene-d_8, 25 °C):



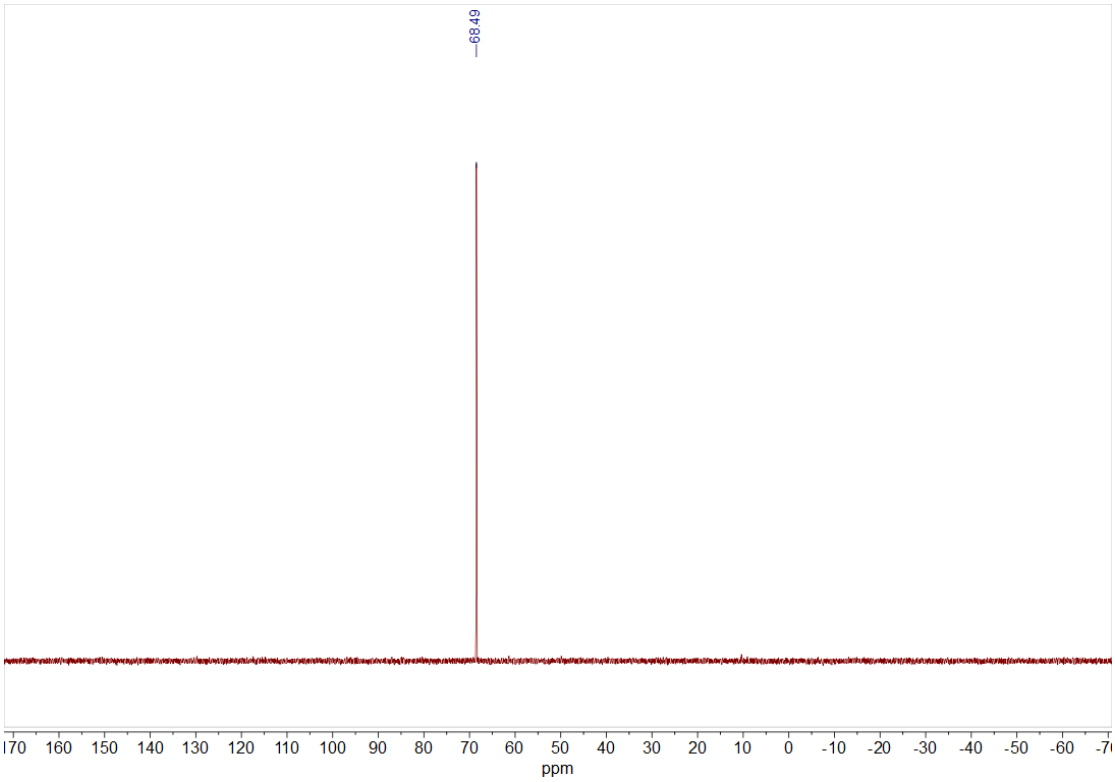
HMBC (^{13}C, ^{1}H) (Toluene-d_8, 25 ^{o}C):



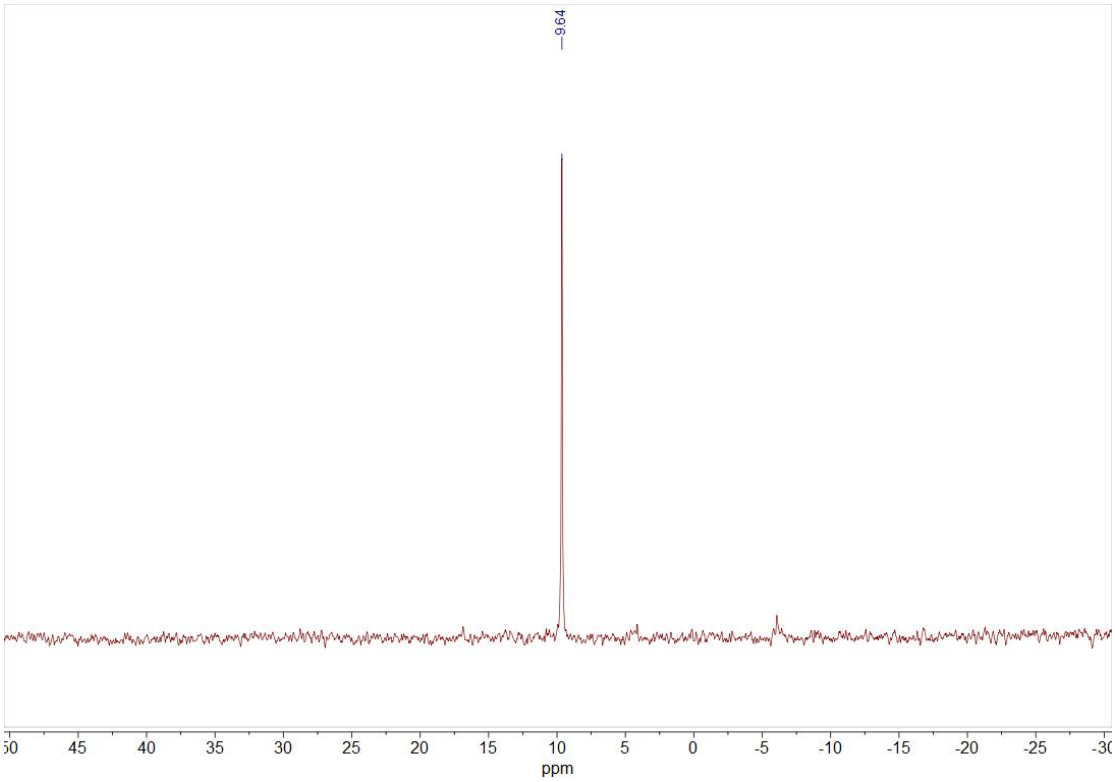
HMQC (^{31}P, ^{13}C) (Toluene-d_8, 25 ^{o}C):



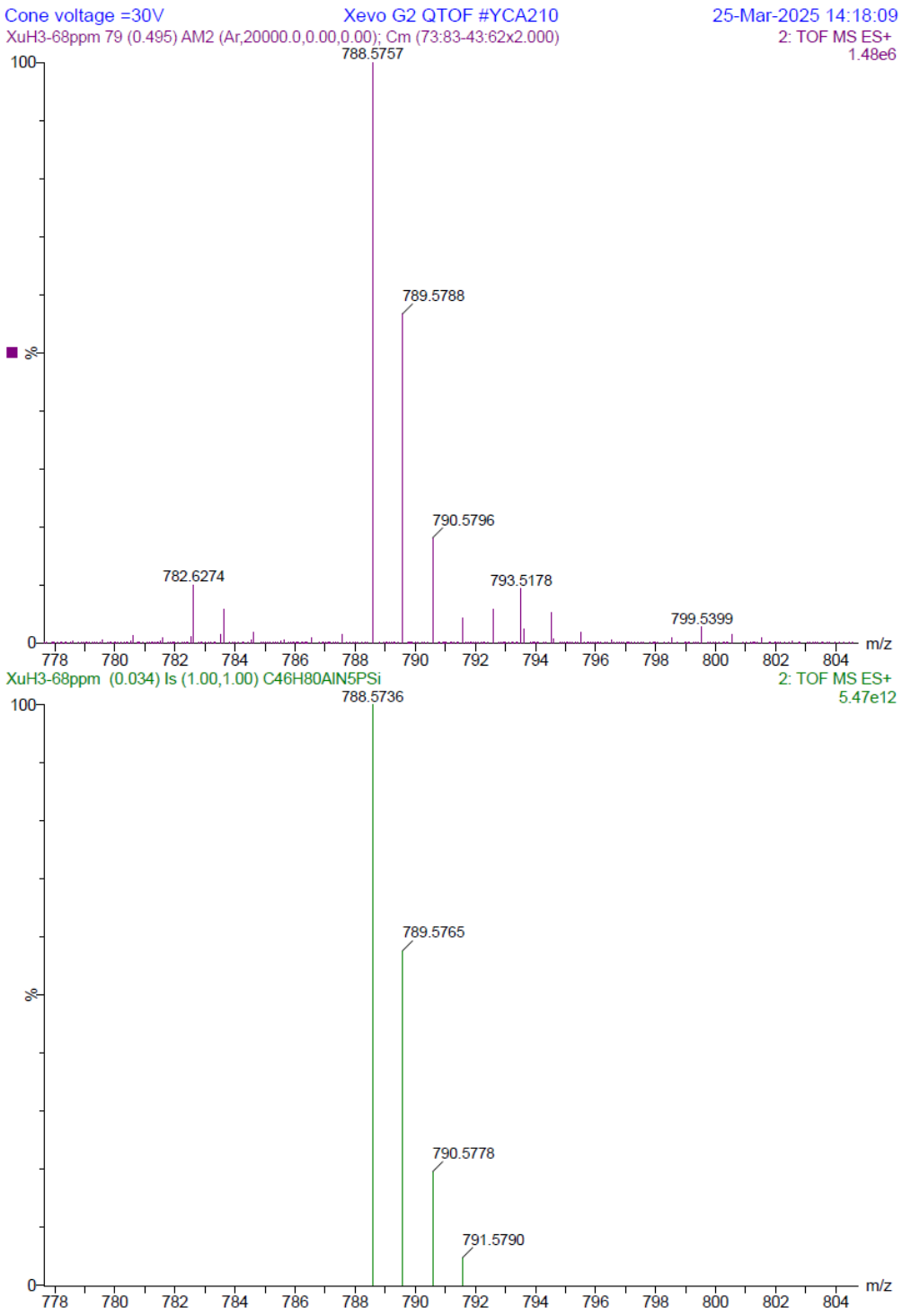
$^{31}P\{^{1}H\}$ NMR (121 MHz, Toluene-d_8, 25 °C):

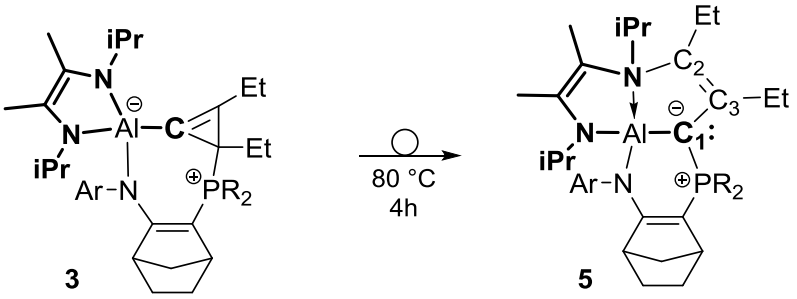


$^{29}Si\{^{1}H\}$ NMR (99 MHz, Toluene-d_8, 25 °C):



HRMS spectra of 3 (top: observed, bottom: simulated):





Synthesis of 5: The solution of **3** (0.2 g, 0.254 mmol) in toluene (5 ml) was heated at 80 °C with 4 hours. The color of solution became yellow from brown. After cooling the solution to room temperature, all volatiles were removed under vacuum. The residue was extracted with pentane (3 X 5 ml). Then the solution was concentrated to 4 ml and was stored at –25 °C overnight to obtain **5** as yellow crystals (0.17 g, yield = 85 %). Mp: 198-200 °C (decomp.).

^{1}H NMR (400 MHz, Toluene-d_8, 25 °C): δ 0.47 (s, 3H, $SiCH_3$), 0.49 (br, 3H, CH_{3NiPr}), 0.50 (s, 3H, $SiCH_3$), 1.03 – 0.94 (br, 3+1H, CH_{3NiPr}+CH_2), 1.08 (t, J_{HH} = 7.2 Hz, 3H, CH_{3Et}), 1.11 (d, J_{HH} = 6.2 Hz, 3H, CH_{3NiPr}), 1.17 (d, J_{HH} = 6.7 Hz, 3H, CH_{3iPr}), 1.20 (d, J_{HH} = 6.9 Hz, 3H, CH_{3iPr}), 1.21 (d, J_{HH} = 6.7 Hz, 3H, CH_{3iPr}), 1.24 (d, J_{HH} = 6.7 Hz, 3H, CH_{3iPr}), 1.37 (s, 9H, CH_{3tBu}), 1.41 (d, J_{HH} = 6.6 Hz, 3H, CH_{3NiPr}), 1.43 (m, 2H, CH_2), 1.46 (t, J_{HH} = 7.5 Hz, 3H, CH_{3Et}), 1.49 (s, 9H, CH_{3tBu}), 1.64 (s, 3H+1H, CH_3+CH_2), 1.72 (s, 3H, CH_3), 1.78 (m, 2H, CH_2), 1.82 (m, 1H, CH_{2Et}), 2.49 (m, 1H, CH_{2Et}), 2.56 (m, 2H, CH_{2Et}), 2.73 (s, 1H, $CH_{bridgehead}$), 3.20 (br, 1H, $CH_{bridgehead}$), 3.58 (sept, J_{HH} = 6.5 Hz, 1H, CH_{NiPr}), 3.60 (sept, J_{HH} = 6.7 Hz, 1H, CH_{iPr}), 3.68 (br, 1H, CH_{NiPr}), 4.25 (sept, J_{HH} = 6.8 Hz, 1H, CH_{iPr}), 7.15 – 7.06 (m, 3H, CH_{Ar}).

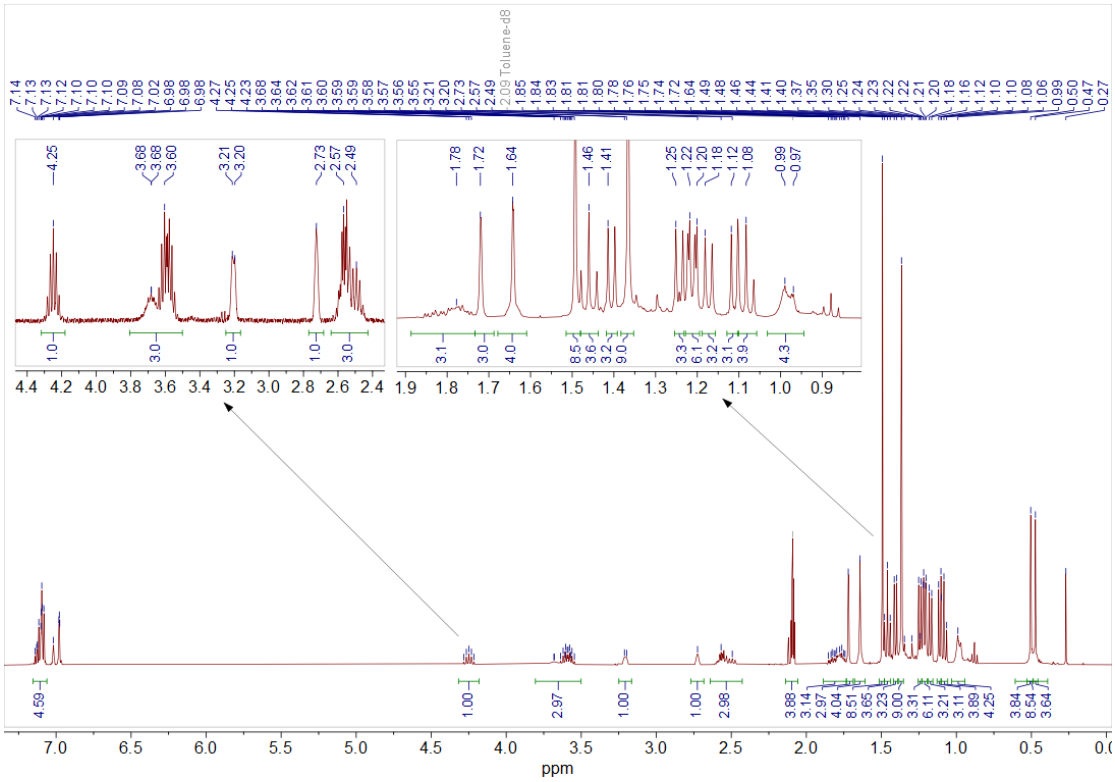
^{13}C{^{1}H} NMR (101 MHz, Toluene-d_8, 25 °C): δ 5.1 (s, $SiCH_3$), 6.1 (d, J_{CP} = 2.5 Hz, $SiCH_3$), 14.0 (s, CH_3), 16.6 (s, CH_{3Et}), 16.8 (d, J_{CP} = 1.8 Hz, CH_{3Et}), 18.0 (br, CH_3), 19.9 (s, CH_{3NiPr}), 21.7 (s, CH_{3NiPr}), 23.9 (br, CH_{2Et}), 24.8 (s, CH_{3iPr}), 25.7 (s, CH_{3NiPr}), 26.1 (s, CH_{3NiPr}), 26.5 (s, CH_{3iPr}), 26.8 (s, CH_{3iPr}), 26.9 (s, CH_{iPr} + CH_2), 27.0 (d, J_{CP} = 13.5Hz, CH_{2Et}), 27.6 (s, CH_{3iPr}), 28.0 (s, CH_{iPr}), 31.4 (s, CH_2), 33.2 (d, J_{CP} = 4.5 Hz, CH_{3tBu}), 34.5 (d, J_{CP} = 4.6 Hz, CH_{3tBu}), 43.9 (d, J_{CP} = 13.1 Hz, $CH_{bridgehead}$), 45.5 (d, J_{CP} = 5.2 Hz, CH_2), 46.4 (s, CH_{NiPr}), 47.8 (d, J_{CP} = 12.7 Hz, $CH_{bridgehead}$), 50.9 (s, CH_{NiPr}), 51.5 (s, C_{tBu}), 52.3 (s, C_{tBu}), 56.1 (br, J_{CP} = 115.1 Hz, detected by hmbc (^{31}P, ^{13}C), Al-C_1), 102.5 (d, J_{CP} = 140.2 Hz, PC), 108.4 (s, Me-C=C), 125.0 (s, CH_{Ar}), 125.1 (s, CH_{Ar}), 125.4 (s, CH_{Ar}), 127.4 (overlapped with toluene signal, J_{CP} = 25.1 Hz, Et-C_3), 145.5 (s, N-C_{Ar}), 146.0 (s, iPr-C_{Ar}), 146.5 (d, J_{CP} = 7.1 Hz, Et-C_2), 146.7 (s, iPr-C_{Ar}), 147.0 (s, Me-C=C), 169.1 (d, J_{CP} = 5.7 Hz, NC).

^{31}P{^{1}H} NMR (162 MHz, Toluene-d_8, 25 °C): δ 10.4 (CP).

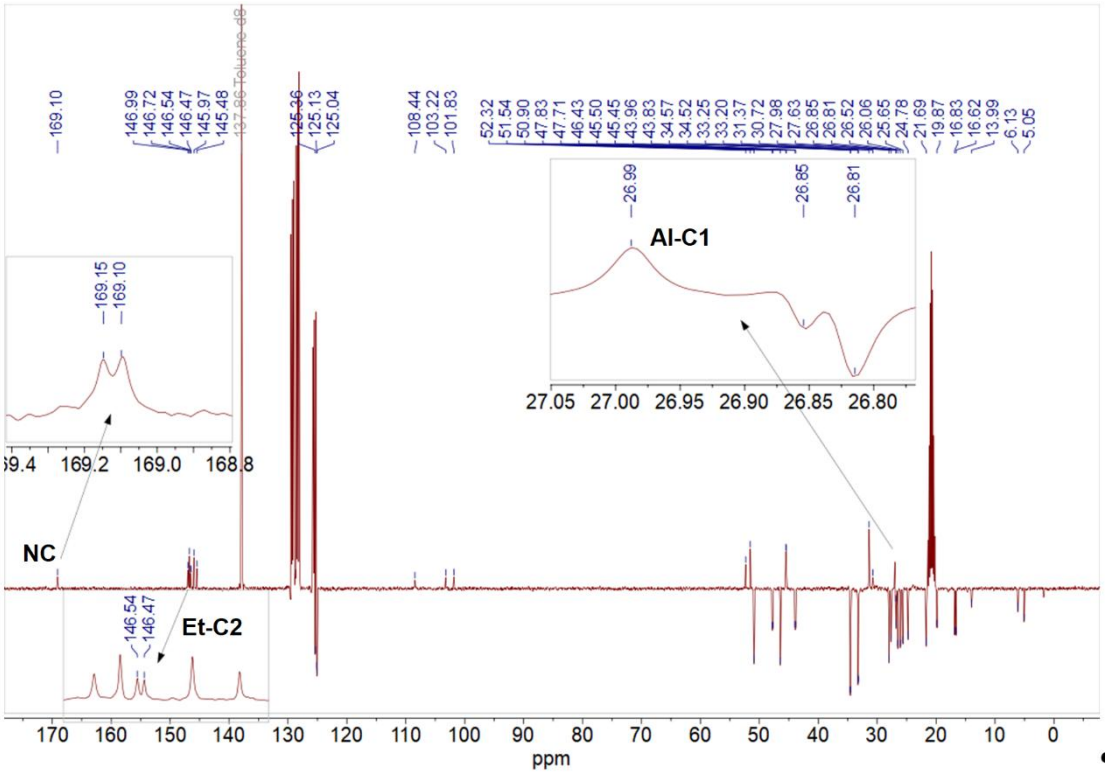
^{29}Si{^{1}H} NMR (80 MHz, Toluene-d_8, 25 °C): δ -6.1 ($SiCH_3$).

HRMS (ESI): m/z $[M]^+$ calcd for $C_{46}H_{80}AlN_5PSi$: 788.5736; found: 788.5750.

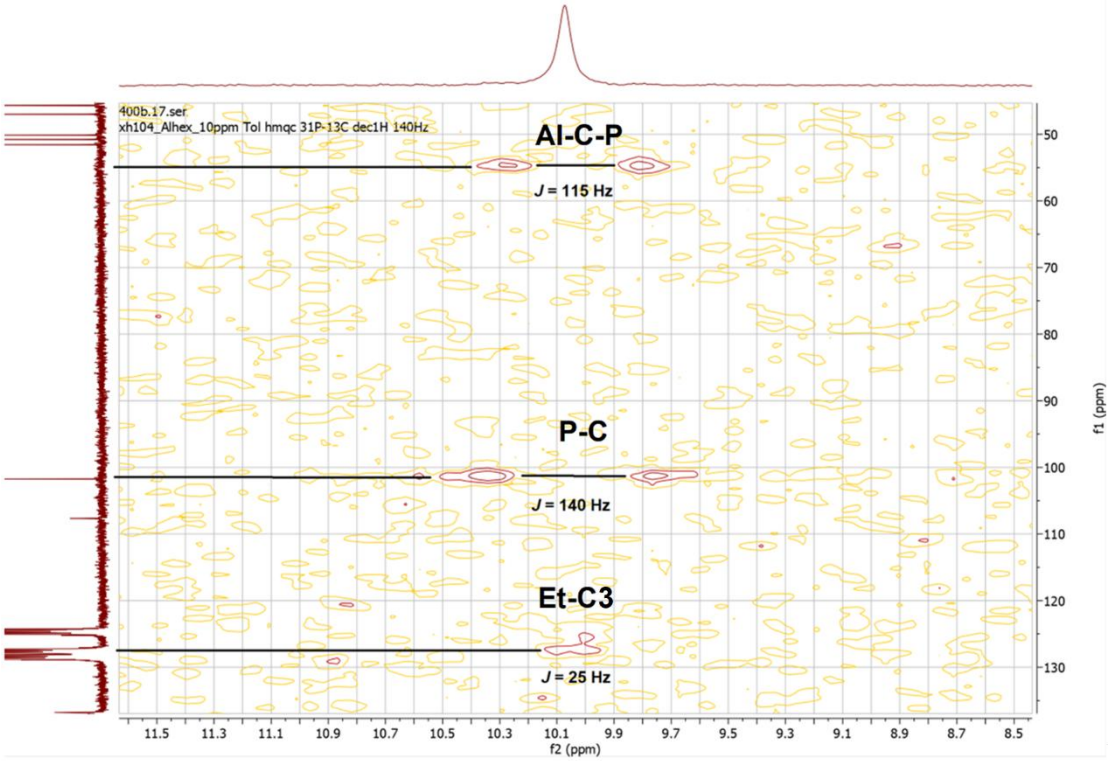
^{1}H NMR (400 MHz, Toluene-d_8, 25 °C):



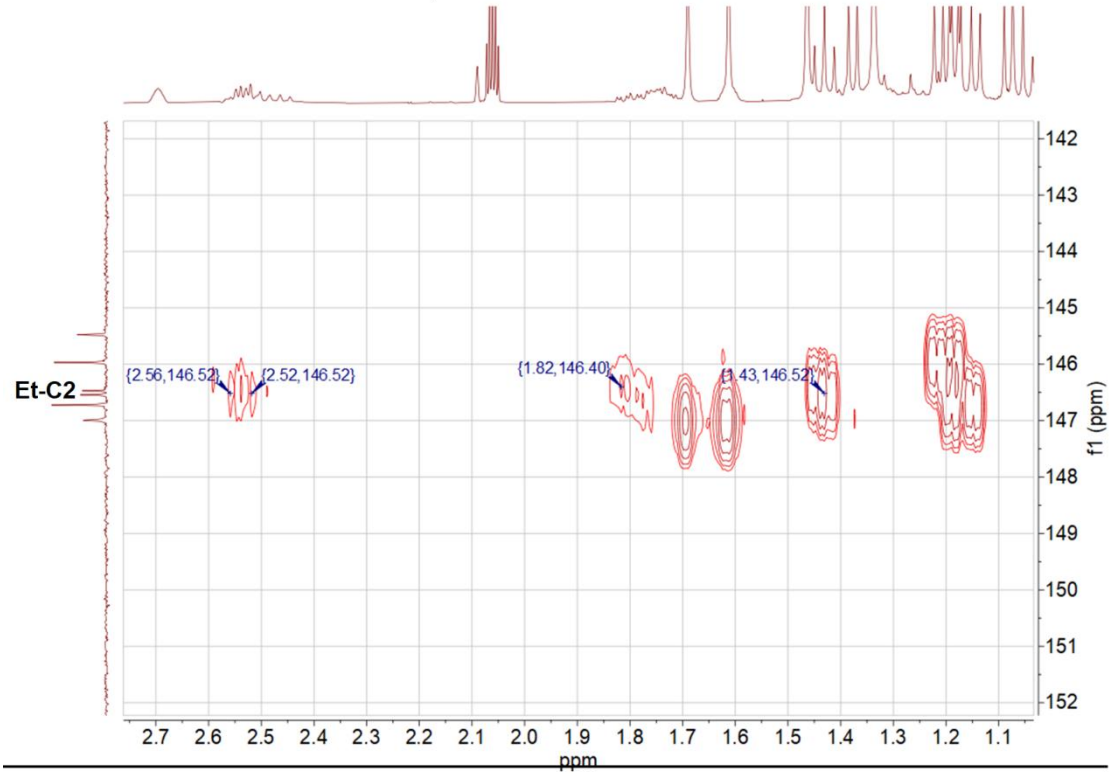
^{13}C{^{1}H} NMR (101 MHz, Toluene-d_8, 25 °C):



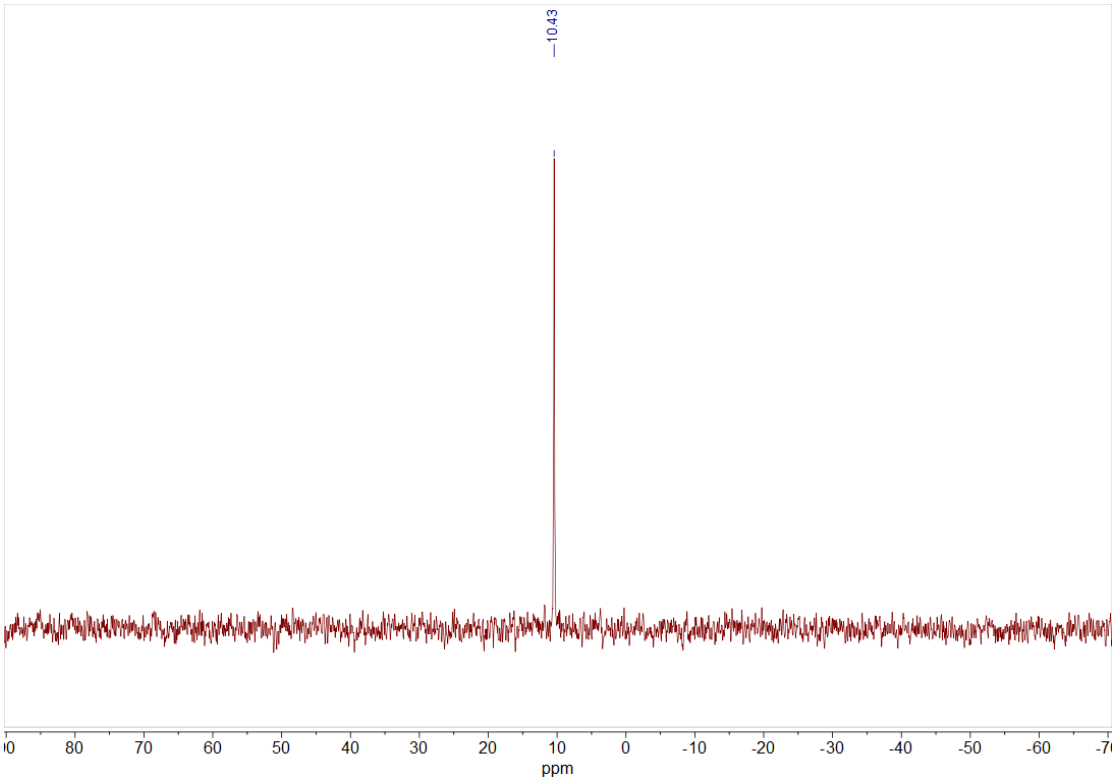
HMBC (^{31}P, ^{13}C) (Toluene-d_8, 25 ^{o}C):



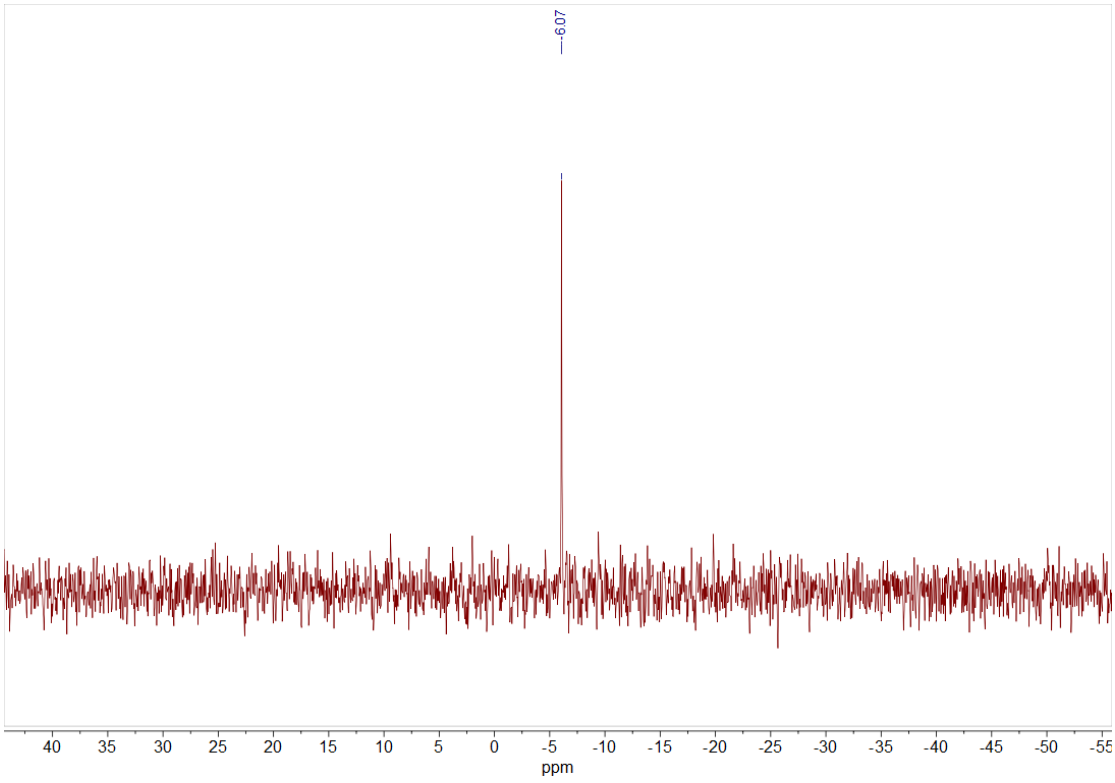
HMBC (^{1}H, ^{13}C) (Toluene-d_8, 25 ^{o}C)



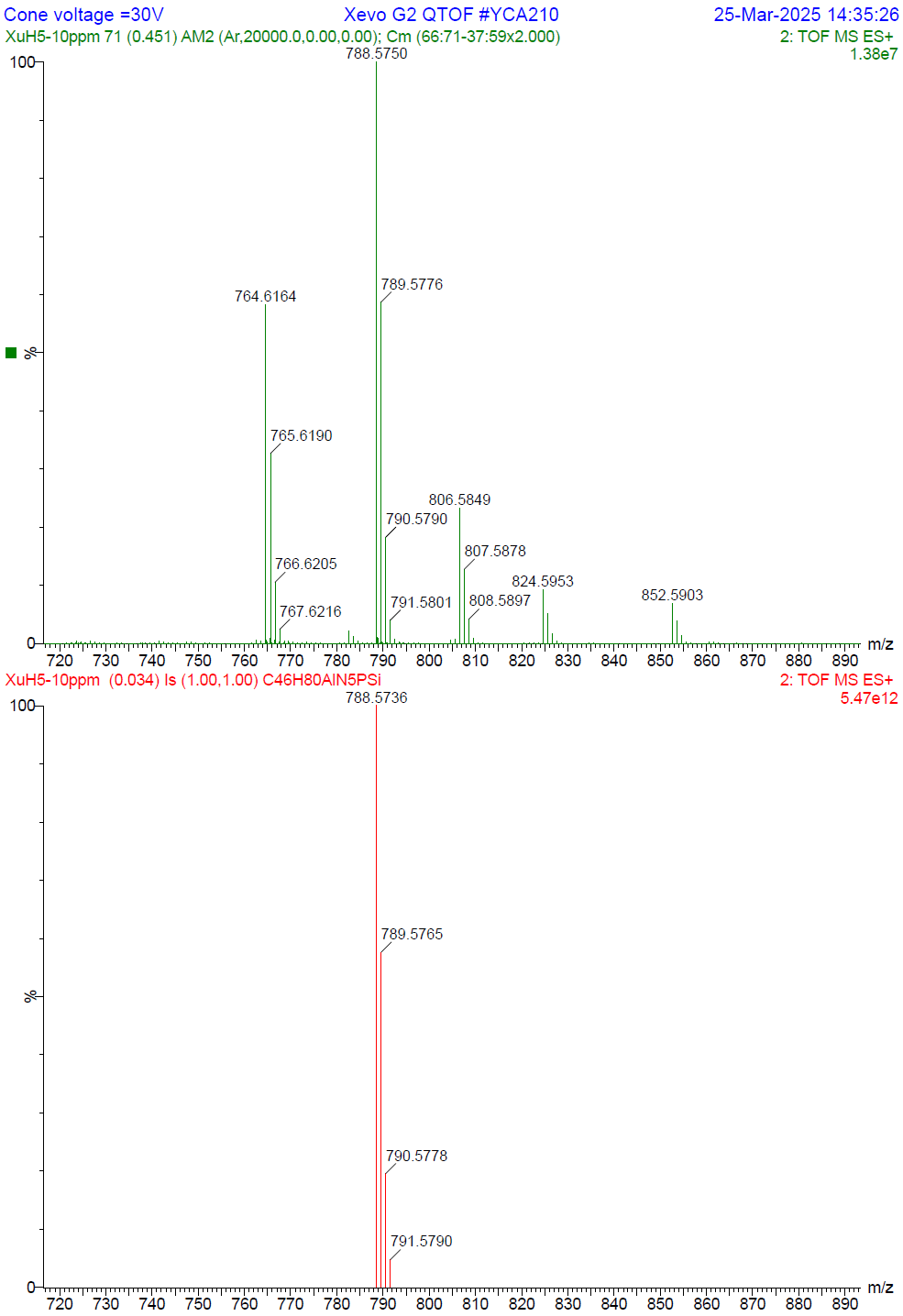
$^{31}P\{^{1}H\}$ NMR (162 MHz, Toluene-d_8, 25 °C):

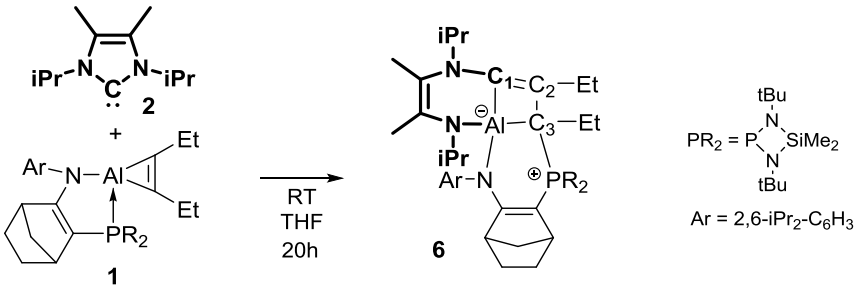


$^{29}Si\{^{1}H\}$ NMR (80 MHz, Toluene-d_8, 25 °C):



HRMS spectra of 5 (top: observed, bottom: simulated):





Synthesis of 6: To a solution of **1** (0.2 g, 0.329 mmol) in toluene (5 ml), NHC (0.06 g, 0.329 mmol) in toluene (2.5 ml) was added at room temperature. After stirring for 20 hours, the solution was filtrated and dried under vacuum. The crude product was extracted by pentane (2 X 5 ml). Then, the solution was concentrated to 2.5 ml and store at –25 °C overnight to obtain **6** as yellow crystals (0.026 g, yield = 10 %). Mp: 205-208°C (decomp.).

^{1}H NMR (500 MHz, THF-d_8, -40 °C): δ 0.56 (s, 3H, $SiCH_3$), 0.63 (s, 3H, $SiCH_3$), 0.77 (d, J_{HH} = 5.9 Hz, 3H, CH_{3NiPr}), 0.82 (s, 3H, C=C-$\underline{C}H_3$), 0.98 (d, J_{HH} = 6.7 Hz, 3H, CH_{3NiPr}), 1.00 (d, J_{HH} = 6.6 Hz, 3H, CH_{3iPr}), 1.06 (d, J_{HH} = 6.7 Hz, 3H, CH_{3iPr}), 1.16 ($m_{overlapped}$, 1H, CH_2), 1.18 ($m_{overlapped}$, 3H, CH_{3Et}), 1.23 ($m_{overlapped}$, 3H, CH_{3NiPr}), 1.25 ($m_{overlapped}$, 3H, CH_{3Et}), 1.28 (d, J_{HH} = 6.8 Hz, 3H, CH_{3NiPr}), 1.31 ($d_{overlapkped}$, 3H, CH_{3iPr}), 1.31 ($d_{overlapped}$, 3H, CH_{3iPr}), 1.37 ($m_{overlapped}$, 1H, CH_2), 1.38 (s, 9H, CH_{3tBu}), 1.41 (s, 3H, C=C-$\underline{C}H_3$), 1.47 (s, 9H, CH_{3tBu}), 1.54 (d, J_{HH} = 8.2 Hz, 1H, CH_2), 1.59 ($m_{overlapped}$, 1H, CH_2), 1.80 ($m_{overlapped}$, 2H, CH_2), 1.86 (m, 1H, CH_{2Et}), 2.20 (m, 1H, CH_{2Et}), 2.34 (m, 1H, CH_{2Et}), 2.58 (m, 1H, CH_{2Et}), 2.62 (br, 1H, $CH_{bridgehead}$), 3.28 (sept, J_{HH} = 6.6Hz, 1H, CH_{iPr}), 3.32 (br, 1H, $CH_{bridgehead}$), 3.39 (m, 1H, CH_{NiPr}), 3.40 (m, 1H, CH_{iPr}), 3.99 (sept, J_{HH} = 6.9 Hz, 1H, CH_{NiPr}), 7.02 – 7.12 (m, 3H, CH_{Ar}).

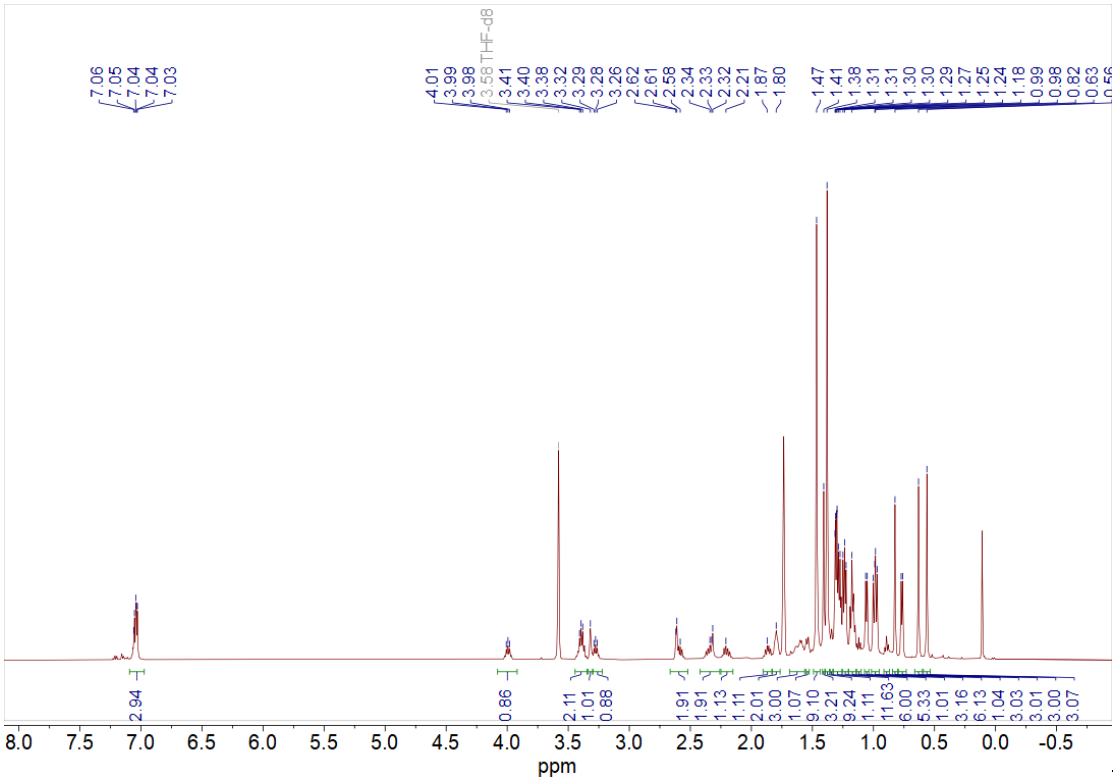
^{13}C{^{1}H} NMR (126 MHz, THF-d_8, -40 °C): δ 4.4 (d, J_{cp} = 2.2 Hz, $SiCH_3$), 6.8 (s, $SiCH_3$), 14.6 (s, CH_{3Et}), 15.4 (d, J_{cp} = 21.3 Hz, CH_{3Et}), 16.7 (s, C=C-$\underline{C}H_3$), 21.7 (s, CH_{3NiPr}), 22.7 (s, C=C-$\underline{C}H_3$), 2.0 (s, CH_{3iPr}), 24.5 (s, CH_{3NiPr}), 25.0 (s, CH_{2Et}), 25.2 (s, CH_{3iPr}), 25.4 (s, CH_{2Et}), 25.8 (s, CH_{3NiPr}), 26.8 (s, CH_2), 27.2 (s, CH_{3iPr}), 27.3 (s, CH_{3NiPr}), 27.5 (s, CH_{3iPr}), 28.5 (s, CH_{iPr}), 28.8 (s, CH_{iPr}), 30.1 (s, CH_2), 33.4 (br, CH_{3tBu}), 33.7 (d, J_{cp} = 3.7 Hz, CH_{3tBu}), 45.4 (d, J_{cp} = 9.5 Hz, $C_{bridgehead}$), 45.9 (d, J_{cp} = 7.8 Hz, CH_2), 46.7 (s, CH_{NiPr}), 48.1 (d, J_{cp} = 11.6 Hz, $C_{bridgehead}$), 50.0 (s, CH_{NiPr}), 52.6 (s, C_{tBu}), 52.7 (s, C_{tBu}), 57.1 (d, J_{cp} = 22.1 Hz, Al-C_3-P), 90.4 (d, J_{cp} = 111.0 Hz, PC), 106.6 (d, J_{cp} = 8.5 Hz, Et-C_2), 123.9 (s, CH_{Ar}), 124.4 (s, Me-C=C), 124.5 (s, CH_{Ar}), 126.0 (s, CH_{Ar}), 133.6 (s, Me-C=C), 143.1 (s, NC_{Ar}), 145.7 (s, iPr-C_{Ar}), 148.1 (s, iPr-C_{Ar}), 178.5 (d, J_{cp} = 10.8 Hz, NC), 178.8 (br, Al-C_1).

^{31}P{^{1}H} NMR (202 MHz, THF-d_8, -40 °C): δ60.3 (CP).

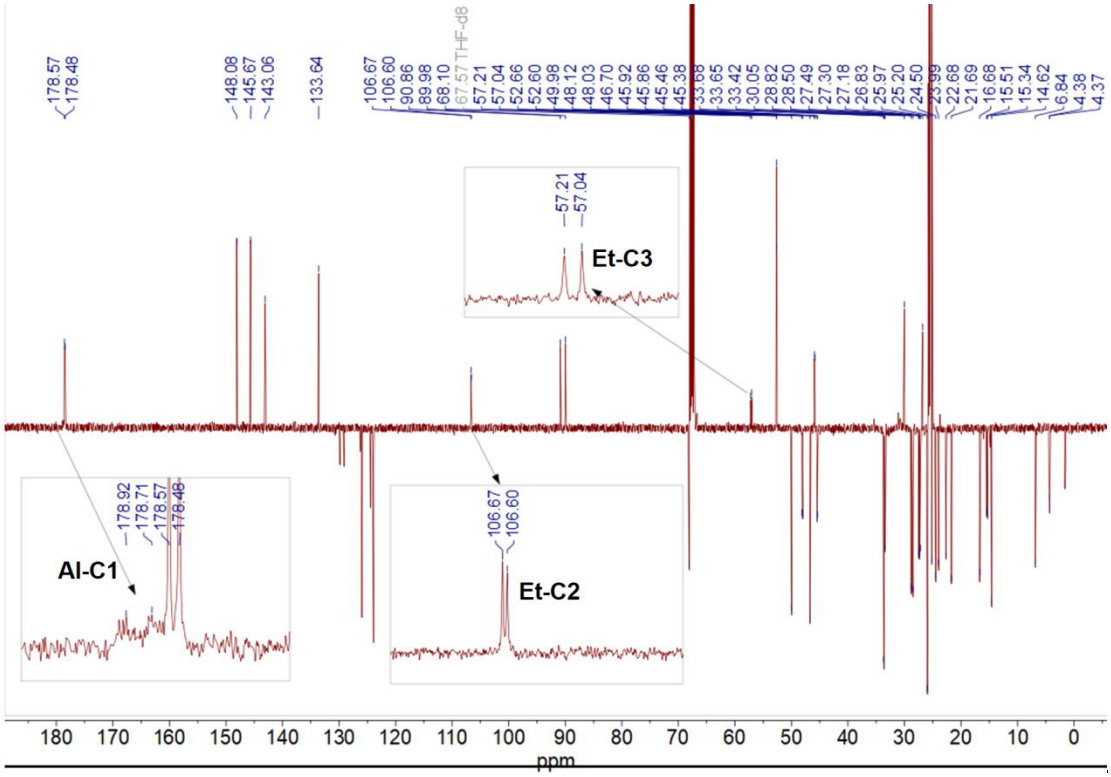
^{29}Si{^{1}H} NMR (99 MHz, THF-d_8, -40 °C): δ9.2 (d, J_{SiP} = 1.2 Hz, $SiCH_3$).

HRMS (ESI): m/z $[M]^+$ calcd for $C_{46}H_{80}AlN_5PSi$: 788.5736; found: 788.5756.

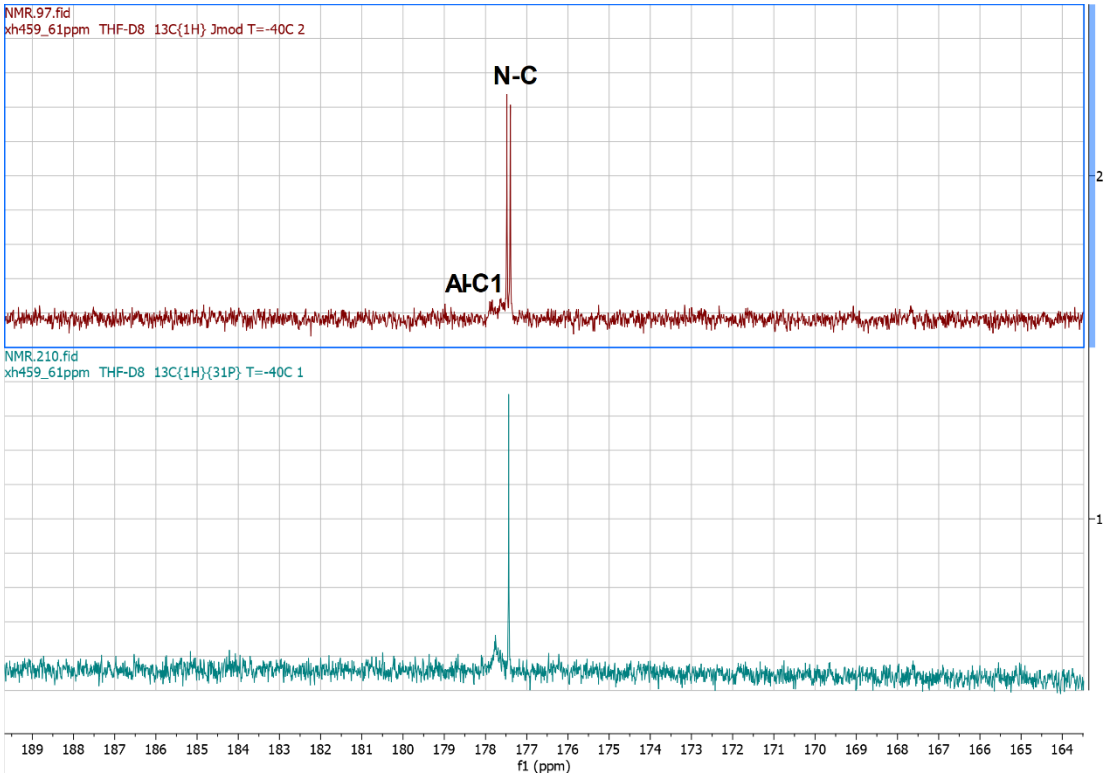
^{1}H NMR (500 MHz, THF-d_8, -40 °C):



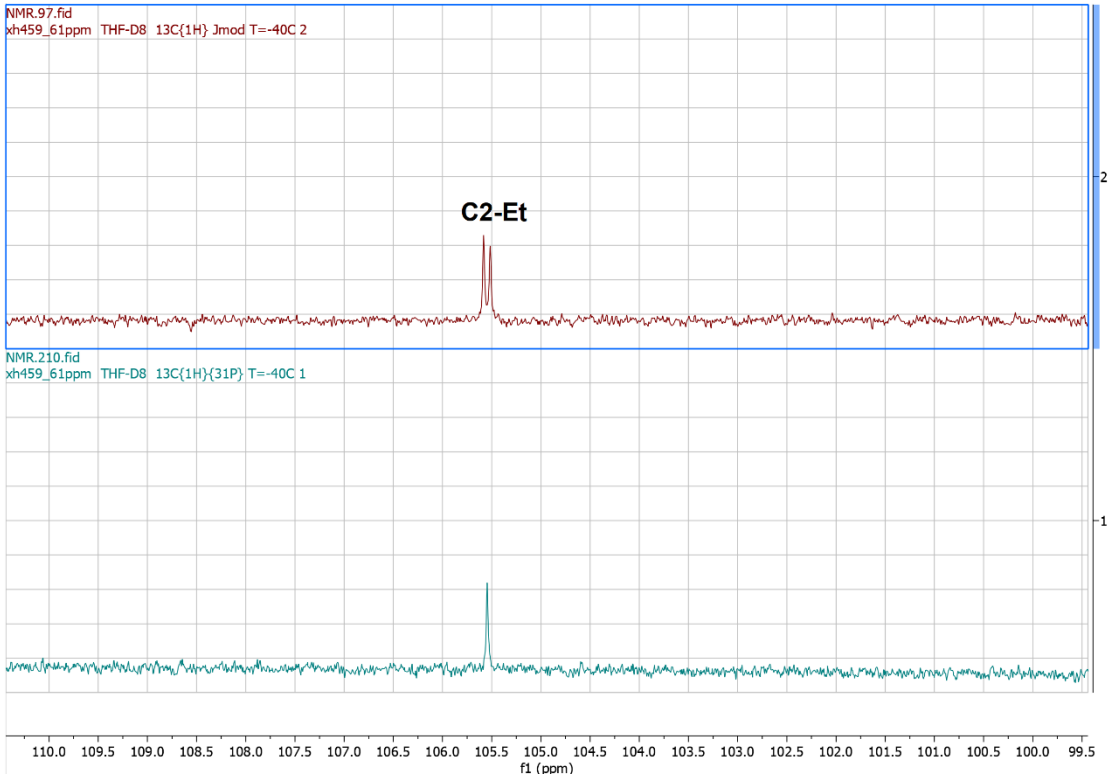
^{13}C{^{1}H} NMR (126 MHz, THF-d_8, -40 °C):



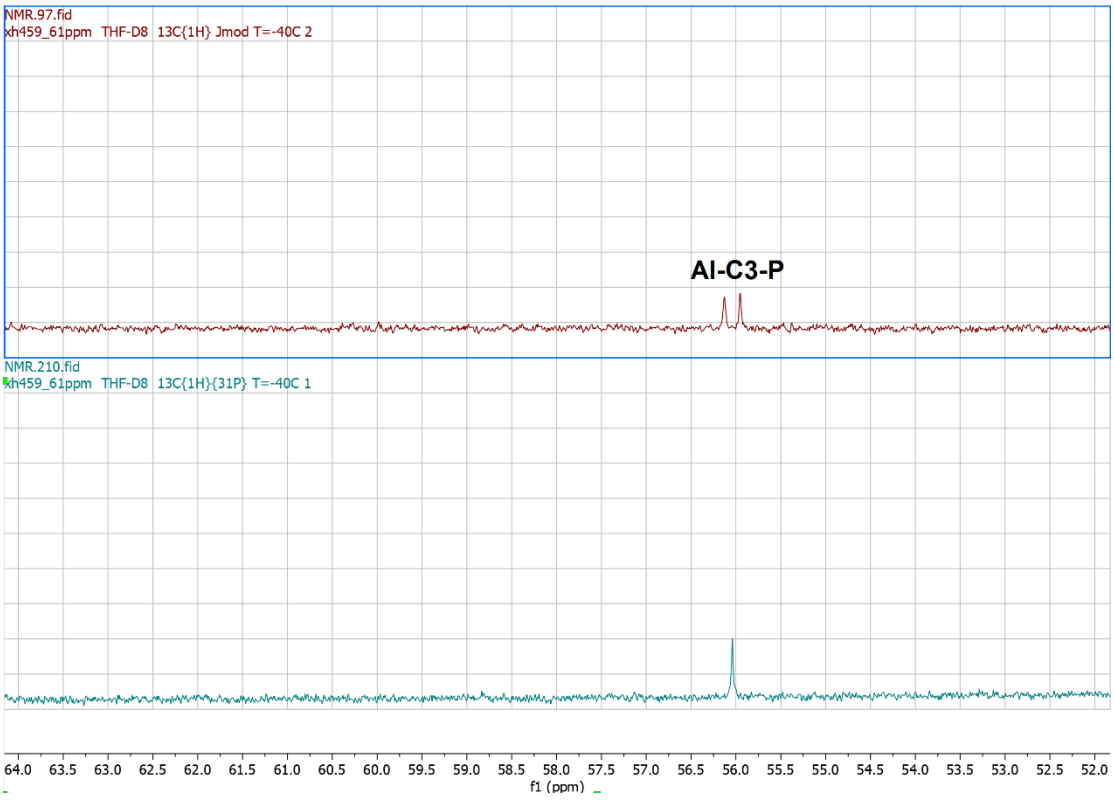
$^{13}C\{^{1}H\}$-NMR (upside) and $^{13}C\{^{1}H,^{31}P\}$-NMR (downside) (500 MHz, THF-d_8, -40 °C):



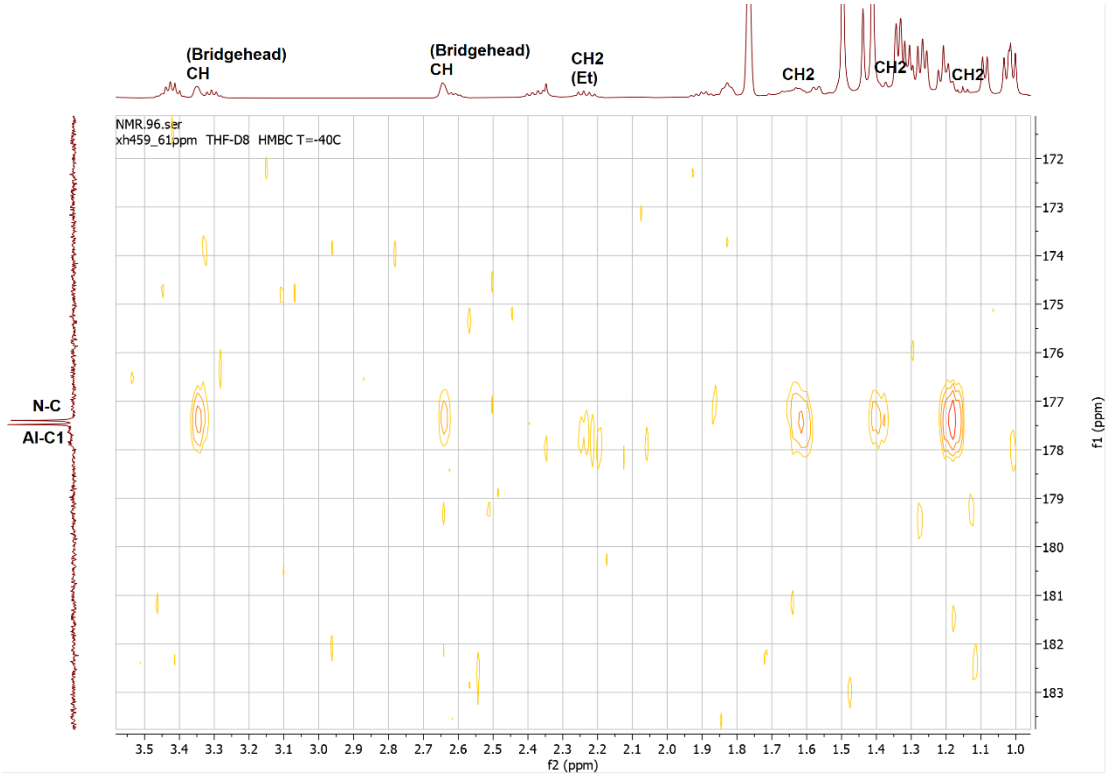
$^{13}C\{^{1}H\}$-NMR (upside) and $^{13}C\{^{1}H,^{31}P\}$-NMR (downside) (500 MHz, THF-d_8, -40 °C):



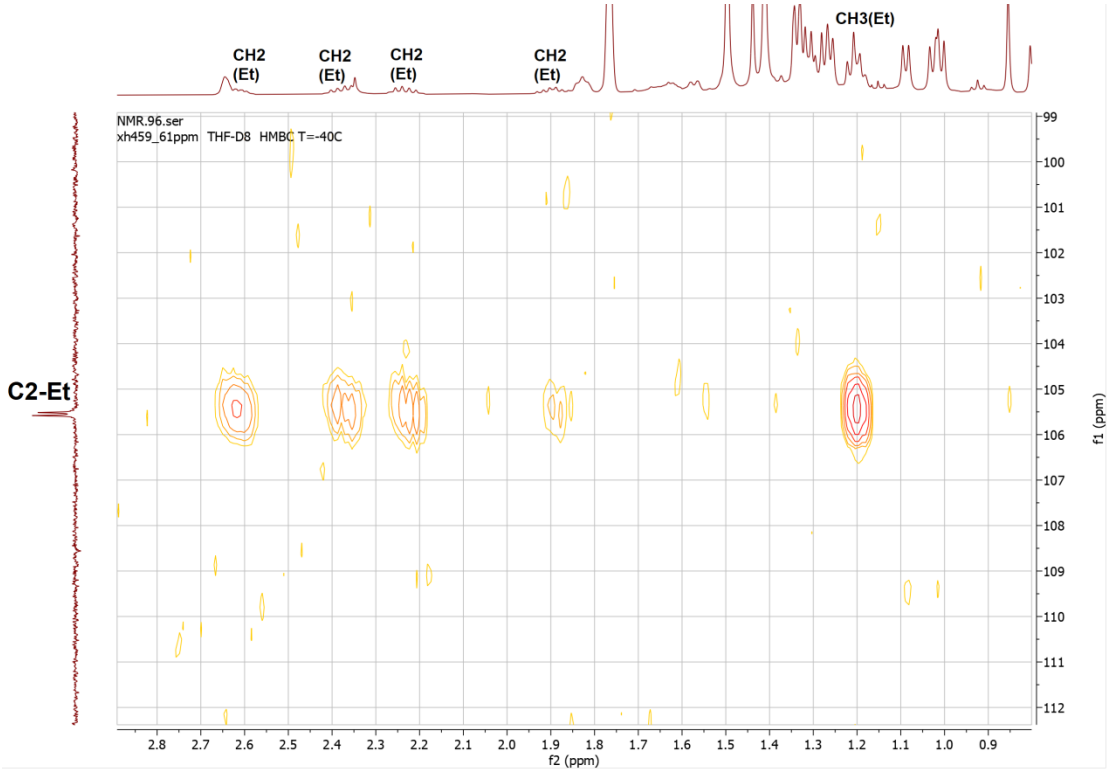
$^{13}C\{^{1}H\}$-NMR (upside) and $^{13}C\{^{1}H,^{31}P\}$-NMR (downside) (500 MHz, THF-d_8, -40 °C):



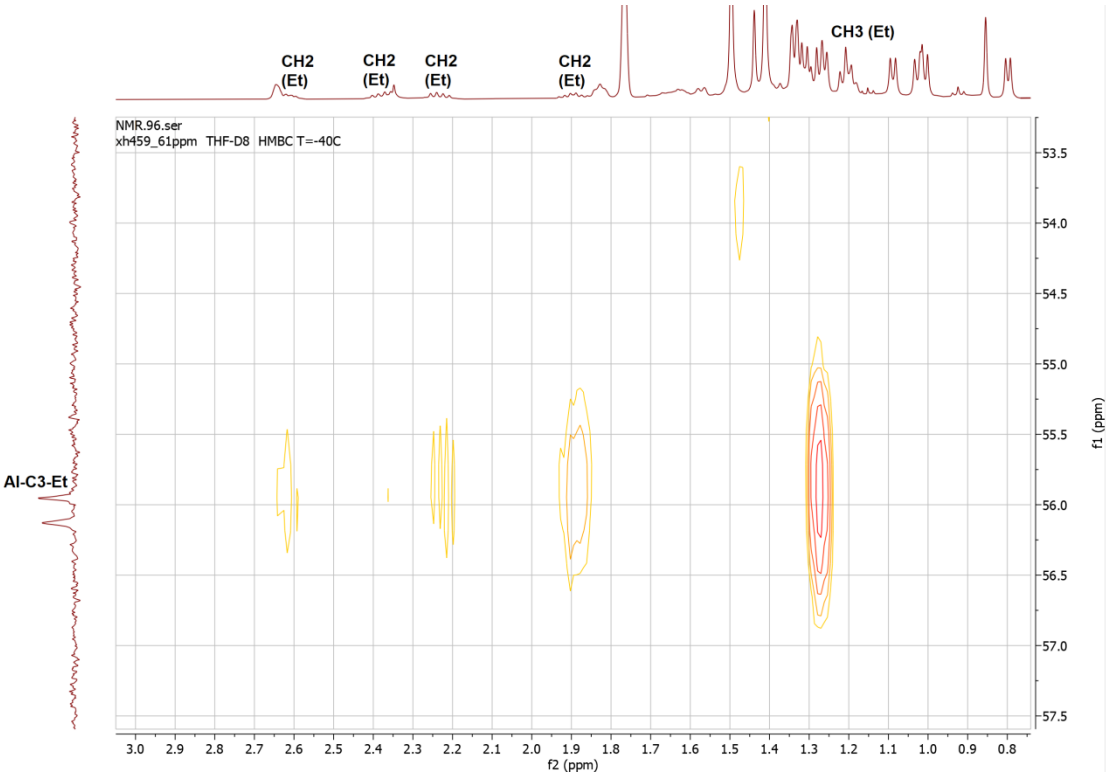
HMBC (^{13}C, ^{1}H) (THF-d_8, -40 °C):



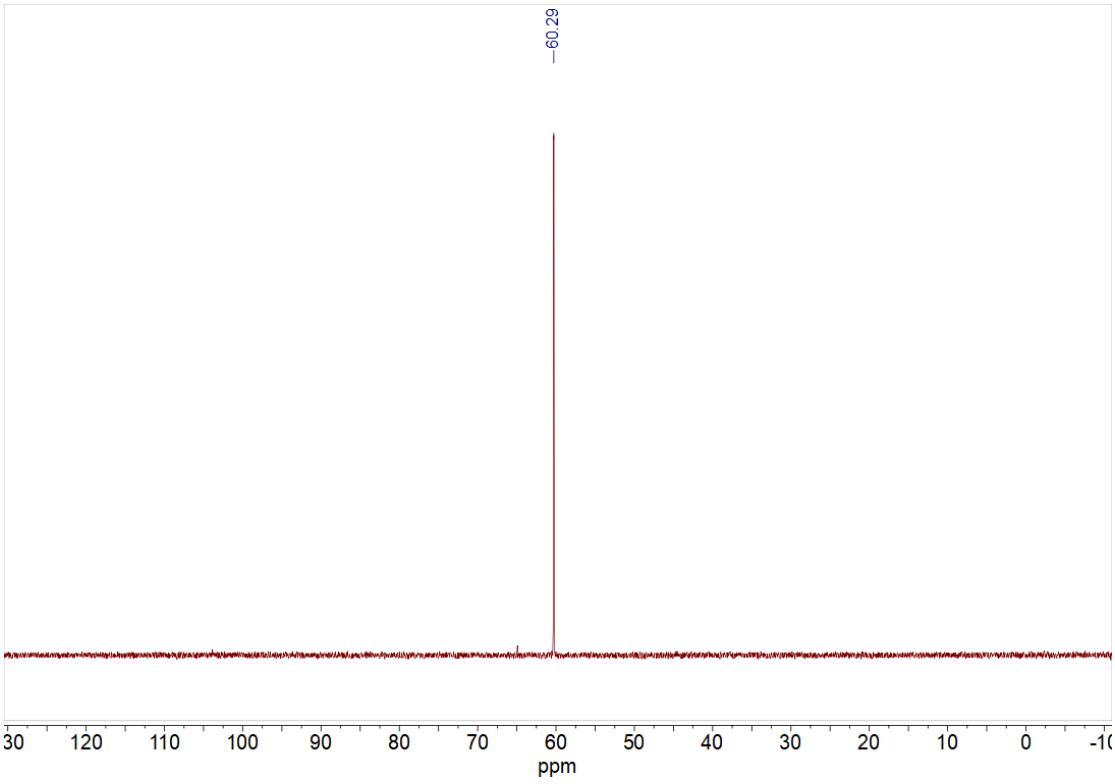
HMBC (^{13}C, ^{1}H) (THF-d_8, -40 ^{o}C):



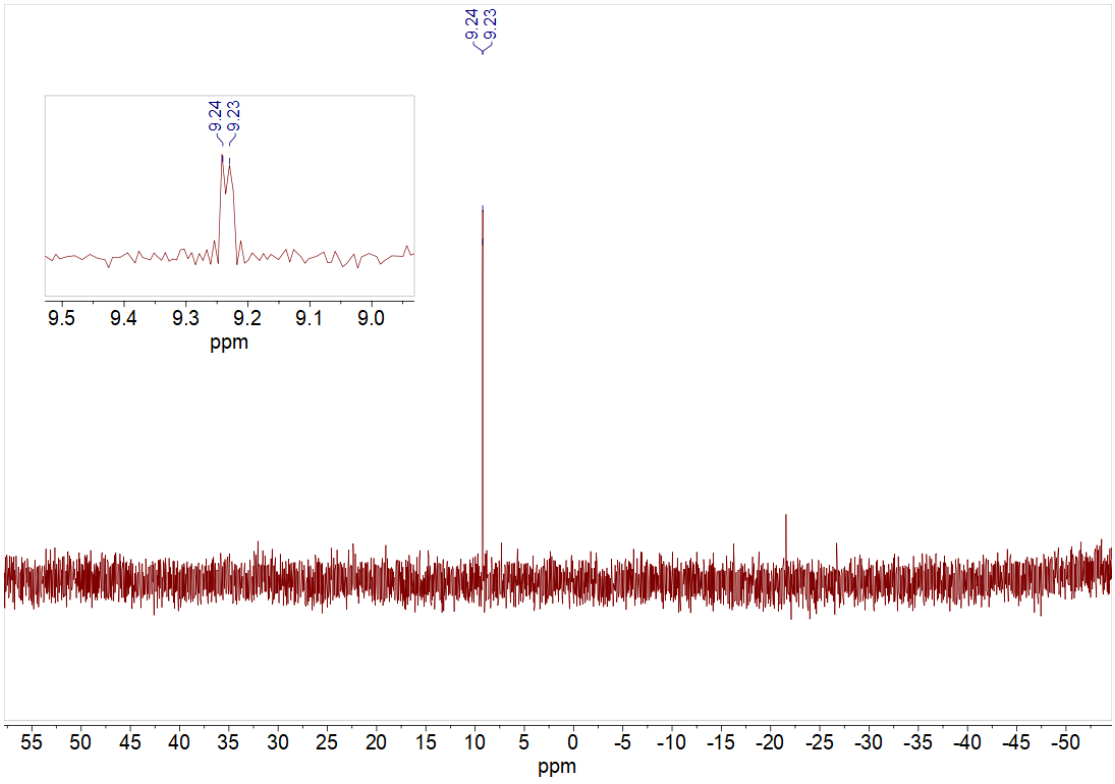
HMBC (^{13}C, ^{1}H) (THF-d_8, -40 ^{o}C):



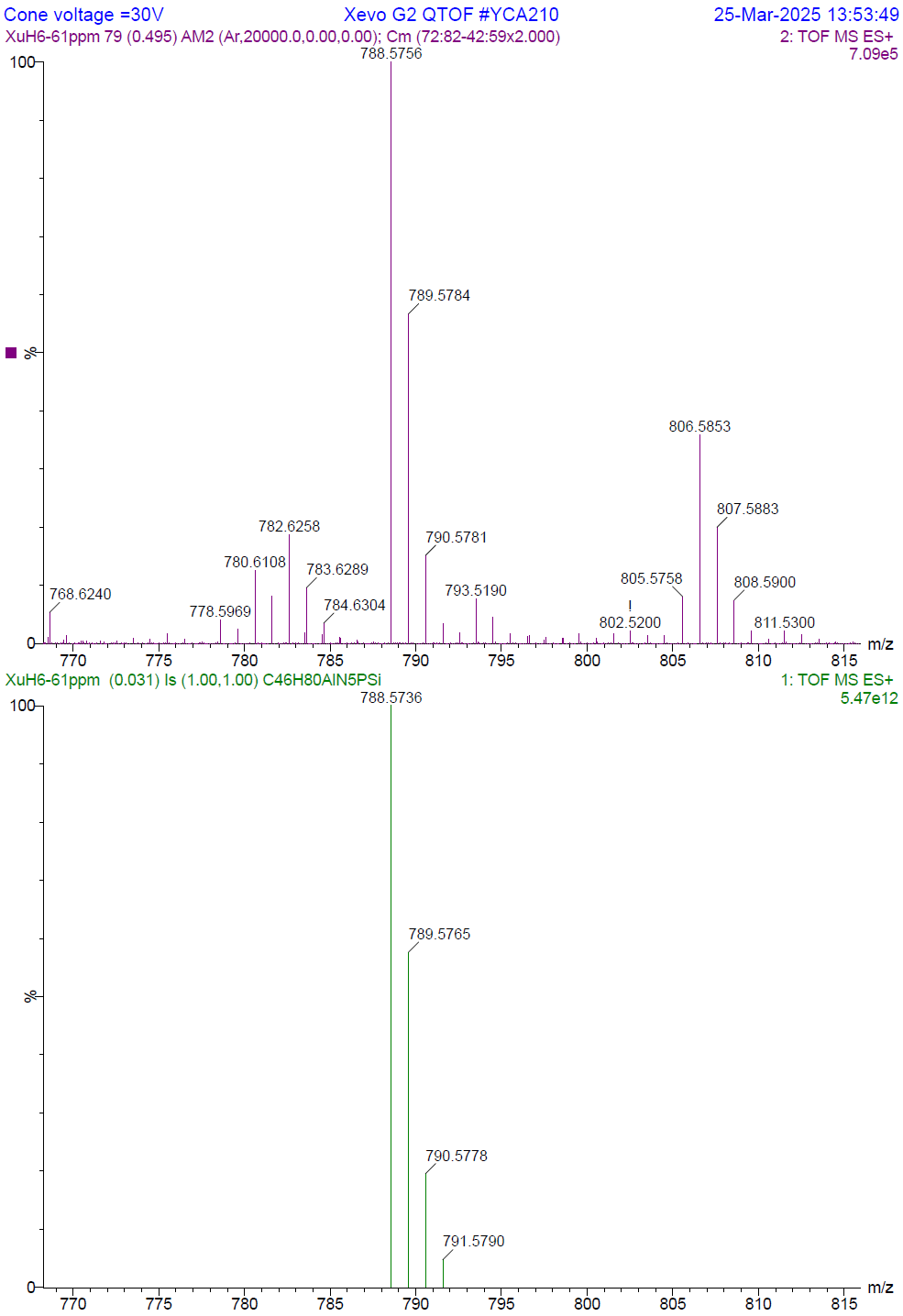
$^{31}P\{^{1}H\}$ NMR (202 MHz, THF-d_8, -40 °C):

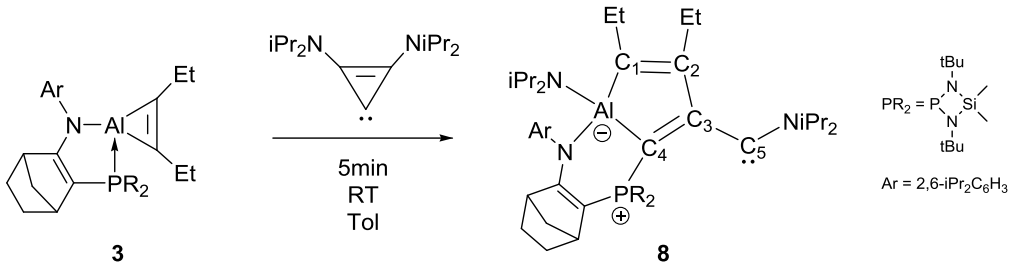


$^{29}Si\{^{1}H\}$ NMR (99 MHz, THF-d_8, -40 °C):



HRMS spectra of 6 (top: observed, bottom: simulated):





Synthesis of 8: To a solution of **3** (200 mg, 0.329 mmol) in toluene (5.0 ml), (diamino)cyclopropylidene (78 mg, 0.329 mmol) in toluene (2.0 ml) was added at room temperature. After 5 min at room temperature, all volatiles were removed under vacuum. The crude products were extracted with pentane (3 x 2 ml), and then the resulting solution was concentrated to 1.0 ml. After overnight at –25 °C, **8** were obtained as red crystals (245 mg, yield = 70 %). Ratio major/minor isomers 85:15. Mp: 100-105 °C (decomp.).

Major diastereomer (85%)

^{1}H NMR (600 MHz, C_6D_6, 25 °C): δ 0.43 (s, 3H, $SiCH_3$), 0.46 (s, 3H, $SiCH_3$), 0.94 (t, J_{HH} = 7.6 Hz, 3H, CH_{3Et}), 0.96 (m, 3H, $CH_{3N\mathit{i}Pr}$), 1.02 (d, J_{HH} = 6.9 Hz, 3H, $CH_{3N\mathit{i}Pr}$), 1.14 (t, J_{HH} = 7.4 Hz, 3H, CH_{3Et}), 1.18 (d, J_{HH} = 6.5 Hz, 3H, $CH_{3N\mathit{i}Pr}$), 1.23 (m, 1H, CH_2), 1.26 [m, 6H, 3H ($CH_{3N\mathit{i}Pr}$) + 3H ($CH_{3\mathit{i}Pr}$)], 1.31 (s, 9H, $CH_{3\mathit{t}Bu}$), 1.34 (m, 3H, $CH_{3\mathit{i}Pr}$), 1.38 (d, J_{HH} = 6.6 Hz, 6H, $CH_{3AlN\mathit{i}Pr}$), 1.41 (m, 1H,CH_2), 1.44 (d, J_{HH} = 6.3 Hz, 6H, $CH_{3AlN\mathit{i}Pr}$), 1.48 (d, J_{HH} = 6.8Hz, 3H, $CH_{3\mathit{i}Pr}$), 1.54 (s, 9H, $CH_{3\mathit{t}Bu}$), 1.63 (d, J_{HH} = 6.5 Hz, 3H, $CH_{3\mathit{i}Pr}$), 1.66 (m, 1H, CH_2), 1.73 (m, 1H, CH_{2Et}), 1.74 (m, 1H, CH_2), 1.88 (m, 1H, CH_2), 2.00 (m, 1H, CH_2), 2.37 (m, 1H, CH_{2Et}), 2.45 (m, 1H, CH_{2Et}), 2.56 (m, 1H, CH_{2Et}), 2.95 (m, 1H, $CH_{bridgehead}$), 3.17 (m, 1H, $CH_{bridgehead}$), 3.43 (hept, J_{HH} = 6.5 Hz, 1H, $CH_{N\mathit{i}Pr}$), 3.57 (m, 1H, $CH_{\mathit{i}Pr}$), 3.82 (hept, J_{HH} = 6.7 Hz, 2H, $CH_{AlN\mathit{i}Pr}$), 4.07 (hept, J_{HH} = 6.6 Hz, 1H, $CH_{N\mathit{i}Pr}$), 4.54 (hept, J_{HH} = 6.7 Hz, 1H, $CH_{\mathit{i}Pr}$), 7.20 – 7.25 (m, 1H, CH_{Ar}), 7.26 (dd, J_{HH} = 7.6 Hz, J_{PH} = 1.9 Hz, 1H, CH_{Ar}), 7.35 (dd, J_{HH} = 7.5 Hz, J_{PH} = 1.9 Hz, 1 H, CH_{Ar}).

^{13}C{^{1}H} NMR (151 MHz, C_6D_6, 25 °C): δ 5.6 (s, $SiCH_3$), 6.1 (d, J_{CP} = 1.4 Hz, $SiCH_3$), 13.9 (s, CH_{3Et}), 16.2 (s, CH_{3Et}), 19.4 (s, $CH_{3AlN\mathit{i}Pr}$), 21.3 (s, $CH_{3AlN\mathit{i}Pr}$), 24.5 (s, CH_{2Et}), 24.9 (s, $CH_{3AlN\mathit{i}Pr}$), 25.0 (s, $CH_{3\mathit{i}Pr}$), 25.5 (s, CH_{2Et}), 25.6 (s, $CH_{3\mathit{i}Pr}$), 25.7 (s, $CH_{3\mathit{i}AlNPr}$), 26.2 (s, CH_2), 26.6 (s, $CH_{3\mathit{i}Pr}$), 26.9 (s, $CH_{3\mathit{i}Pr}$), 27.5 (s, $CH_{\mathit{i}Pr}$), 27.6 (s, $CH_{\mathit{i}Pr}$), 28.0 (s, $CH_{3N\mathit{i}Pr}$ x 2), 28.3 (s, $CH_{3N\mathit{i}Pr}$ x 2), 29.2 (s, CH_2), 33.0 (d, J_{CP} = 4.7 Hz, $CH_{3\mathit{t}Bu}$), 33.3 (d, J_{CP} = 4.7 Hz, $CH_{3\mathit{i}Bu}$), 45.4 (d, J_{CP} = 13.3 Hz, $CH_{bridgehead}$), 47.0 (d, J_{CP} = 9.5 Hz, CH_2), 48.4 (d, J_{CP} = 12.4 Hz, $CH_{bridgehead}$), 49.4 (s, $CH_{AlN\mathit{i}Pr}$ x 2), 50.9 (s, $CH_{N\mathit{i}Pr}$), 51.6 (s, $C_{\mathit{t}Bu}$), 51.8 (s, $C_{\mathit{t}Bu}$), 63.2 (s, $CH_{N\mathit{i}Pr}$), 95.6 (d, J_{CP} = 150.3 Hz, PC), 102.0 (d, J_{CP} = 58.8 Hz, Al-C_4-P), 124.1 (s, CH_{Ar}), 124.6 (s, CH_{Ar}), 125.8 (s, CH_{Ar}), 145.9 (s, N-C_{Ar}), 146.2 (s, iPr-C_{Ar}), 146.4 (s, iPr-C_{Ar}), 149.7 (d, J_{CP} = 26.8 Hz, Et-C_2), 174.2 (d, J_{CP} = 9.0 Hz, C_3), 174.6 (br, Al-C_1-Et), 180.8 (d, J_{CP} = 8.5 Hz, NC), 296.0 (d, J_{CP} = 26.3 Hz, iPr_2N-C_5).

^{31}P{^{1}H} NMR (243 MHz, C_6D_6, 25 °C): δ 20.1 (s, CP).

^{29}Si{^{1}H} NMR (79 MHz, C_6D_6, 25 °C): δ -0.5 (d, J_{SiP} = 1.8 Hz, $SiCH_3$).

Minor diastereomer (16 %):

^{1}H NMR (600 MHz, C_6D_6, 25 °C): δ 0.36 (s, 3H, $SiCH_3$), 0.45 (s, 3H, $SiCH_3$,), 0.78 (t, J_{HH} = 7.6 Hz, 3H, CH_{3Et}), 0.88 (t, J_{HH} = 7.2 Hz, 3H, CH_{3Et}), 1.03 (m, 3H, $CH_{3N\mathit{i}Pr}$), 1.05 (m, 1H, CH_2), 1.10 (m, 1H, CH_2), 1.11 (m, 3H, $CH_{3N\mathit{i}Pr}$), 1.20 (d, J_{HH} = 6.5 Hz, 3H, $CH_{3N\mathit{i}Pr}$), 1.24 (m, 3H, $CH_{3\mathit{i}Pr}$), 1.28 (d, J_{HH} =

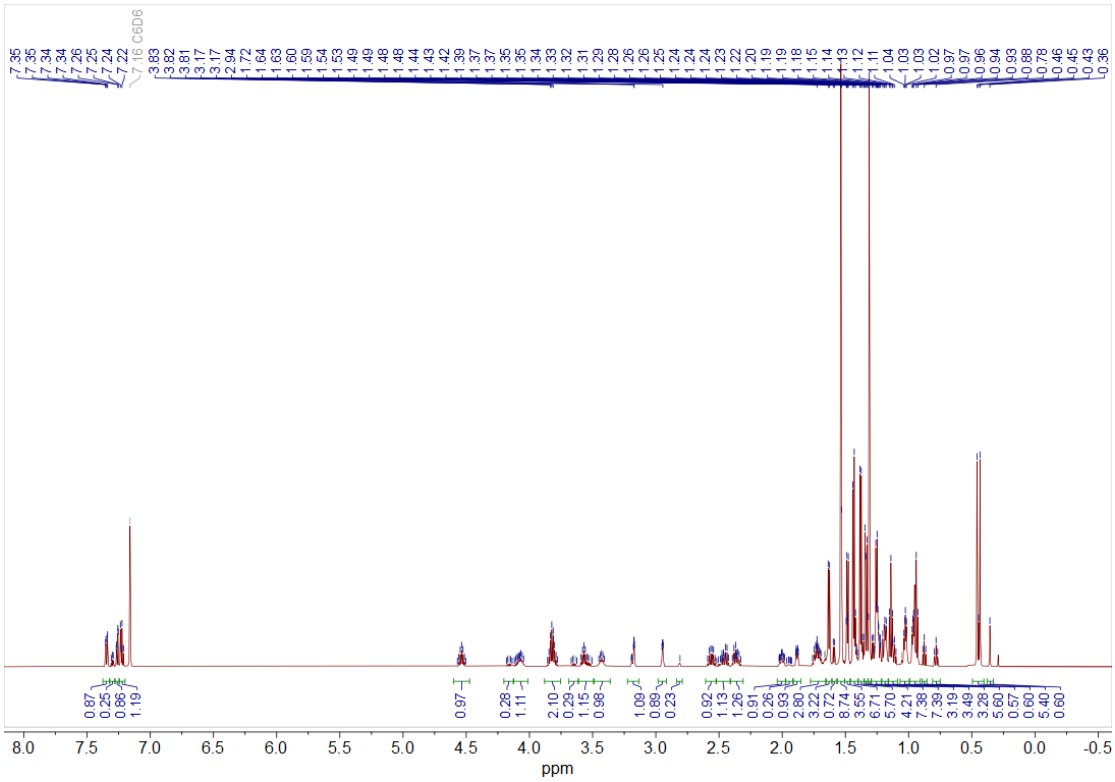
6.6 Hz, 3H, CH_{3iPr}), 1.32 (m, 3H, CH_{3NiPr}), 1.35 (s, 9H, CH_{3tBu}), 1.36 (d, J_{HH} = 6.7 Hz, 3H, CH_{3iPr}), 1.41 (m, 1H, CH_2), 1.42 (m, 6H, $CH_{3AlNiPr}$), 1.49 (d, J_{HH} = 6.8 Hz, 6H, $CH_{3AlNiPr}$), 1.53 (s, 9H, CH_{3tBu}), 1.59 (d, J_{HH} = 6.6 Hz, 3H, CH_{3iPr}), 1.65 (m, 1H, CH_{2Et}), 1.70 (m, 1H, CH_2), 1.95 (m, 1H, CH_2), 2.35 (m, 2H, CH_{2Et}), 2.48 (m, 1H, CH_{2Et}), 2.81 (m, 1H, $CH_{bridgehead}$), 3.19 (m, 1H, $CH_{bridgehead}$), 3.53 (m, 1H, CH_{NiPr}), 3.65 (p, J_{HH} = 6.7 Hz, 1H, CH_{iPr}), 3.80 (sept, J_{HH} = 6.7 Hz, 2H, CH_{AlNiPr}), 4.10 (m, 1H, CH_{NiPr}), 4.16 (sept, J_{HH} = 6.7 Hz, 1H, CH_{iPr}), 7.20 – 7.25 (m, 2H, CH_{Ar}), 7.27 – 7.32 (m, 0.25H, 1 H, CH_{Ar}).

$^{13}C\{^1H\}$ NMR (151 MHz, C_6D_6, 25 °C): δ 5.3 (s, $SiCH_3$), 7.2 (d, J_{CP} = 2.1 Hz, $SiCH_3$), 14.0 (s, CH_{3Et}), 15.4 (s, CH_{3Et}), 19.4 (s, $CH_{3AlNiPr}$), 22.5 (s, $CH_{3AlNiPr}$), 23.3 (s, CH_{2Et}), 25.1 (s, $CH_{3AlNiPr}$), 25.2 (s, CH_{3iPr}), 25.4 (s, CH_{3iPr}), 25.8 (s, $CH_{3AlNiPr}$), 26.6 (s, CH_2), 26.6 (s, CH_{3iPr}), 26.6 (s, CH_{3iPr}), 26.8 (s, CH_{3NiPr}), 27.5 (s, CH_{iPr}), 27.7 (s, CH_{2Et}), 27.7 (s, CH_{iPr}), 28.9 (s, CH_{3NiPr}), 29.3 (s, CH_2), 32.1 (d, J_{CP} = 4.7 Hz, CH_{3tBu}), 34.0 (d, J_{CP} = 5.0 Hz, CH_{3tBu}), 44.9 (d, J_{CP} = 15.2 Hz, $CH_{bridgehead}$), 45.2 (d, J_{CP} = 4.9 Hz, CH_2), 47.6 (d, J_{CP} = 11.9 Hz, $CH_{bridgehead}$), 48.0 (s, CH_{AlNiPr}), 51.5 (s, C_{tBu}), 51.7 (s, CH_{NiPr}), 52.3 (s, C_{tBu}), 61.5 (s, CH_{NiPr}), 96.0 (d, J_{CP} = 147.7 Hz, PC), 102.0 (d, J_{CP} = 58.8 Hz, Al-C_4-P), 124.6 (s, CH_{Ar}), 124.7 (s, CH_{Ar}), 125.6 (s, CH_{Ar}), 145.6 (s, N-C_{Ar}), 146.3 (s, iPr-C_{Ar}), 147.6 (d, J_{CP} = 30.1 Hz, Et-C_2), 148.0 (s, iPr-C_{Ar}), 172.8 (d, J_{CP} = 7.5 Hz, C_3), 175.3 (br, Al-C_1-Et), 180.9 (d, J_{CP} = 8.5 Hz, NC), 301.4 (d, J_{CP} = 16.7 Hz, iPr_2N-C_5).

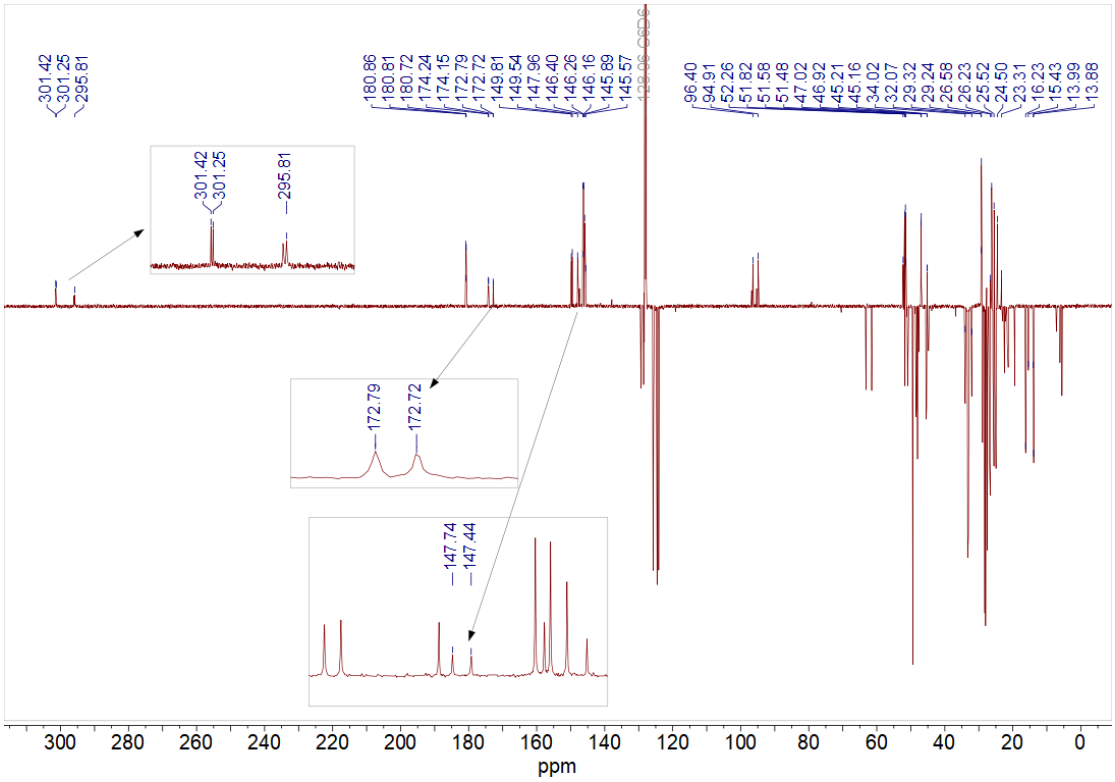
$^{31}P\{^1H\}$ NMR (243 MHz, C_6D_6, 25 °C): δ 26.4 (s, CP)

$^{29}Si\{^1H\}$ NMR (79 MHz, C_6D_6, 25 °C): δ 2.0 (s, $SiCH_3$).

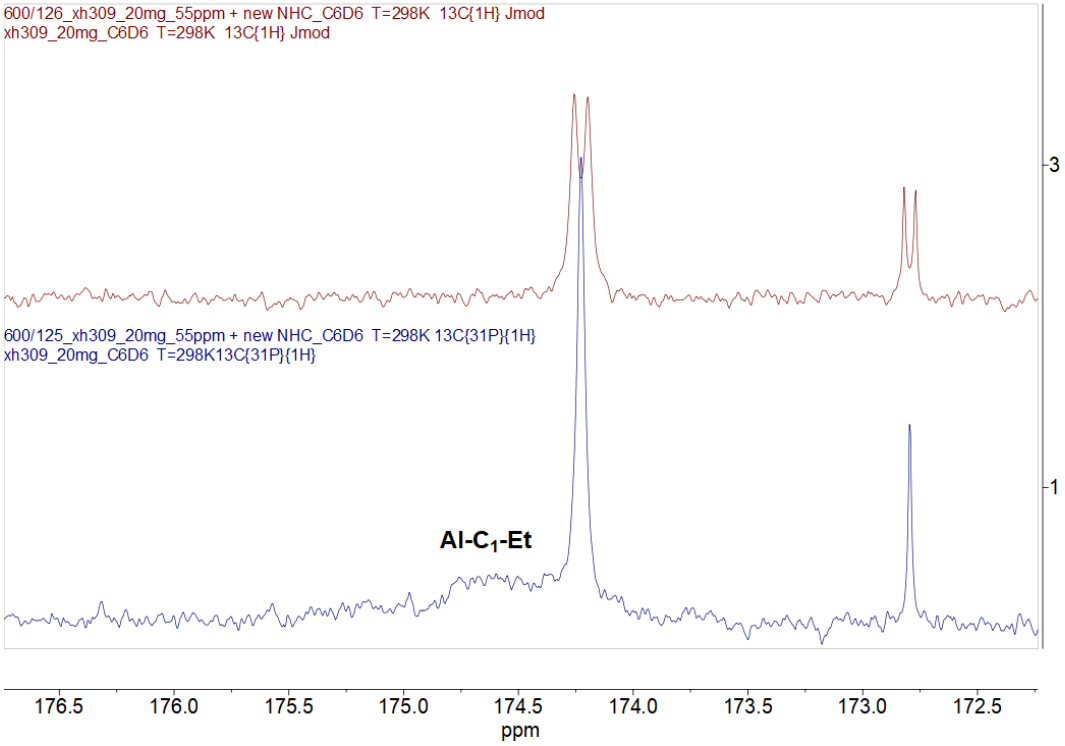
^{1}H NMR (600 MHz, C_6D_6, 25 ^{o}C):



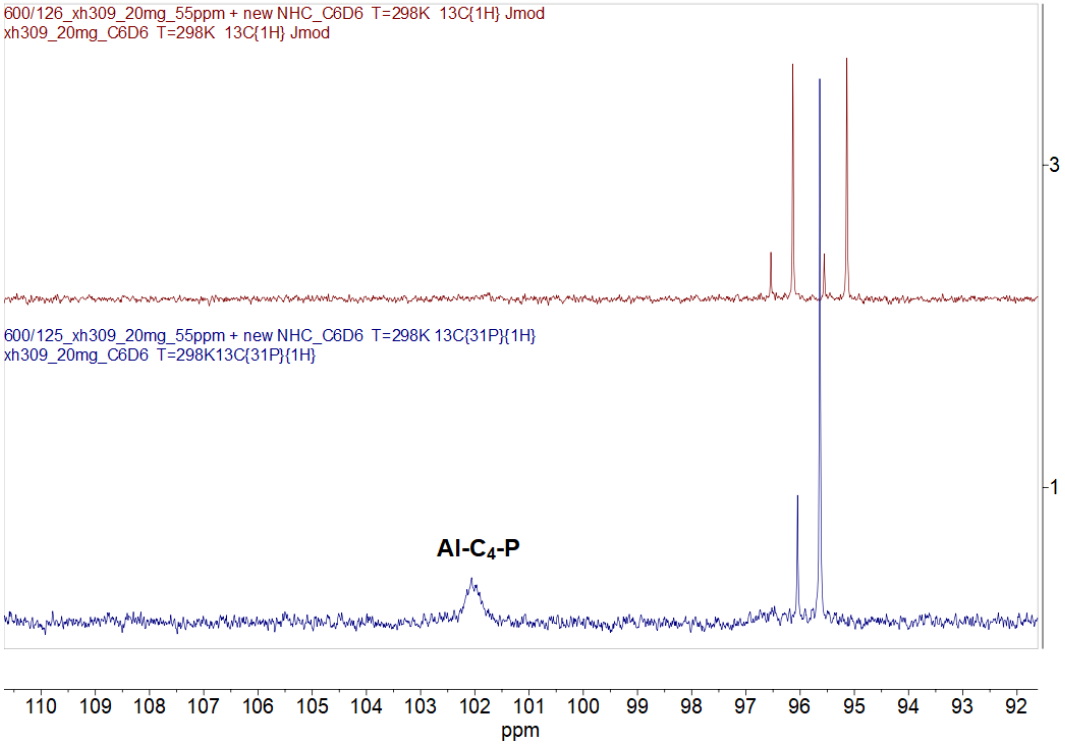
^{13}C{^{1}H} NMR (151 MHz, C_6D_6, 25 ^{o}C):



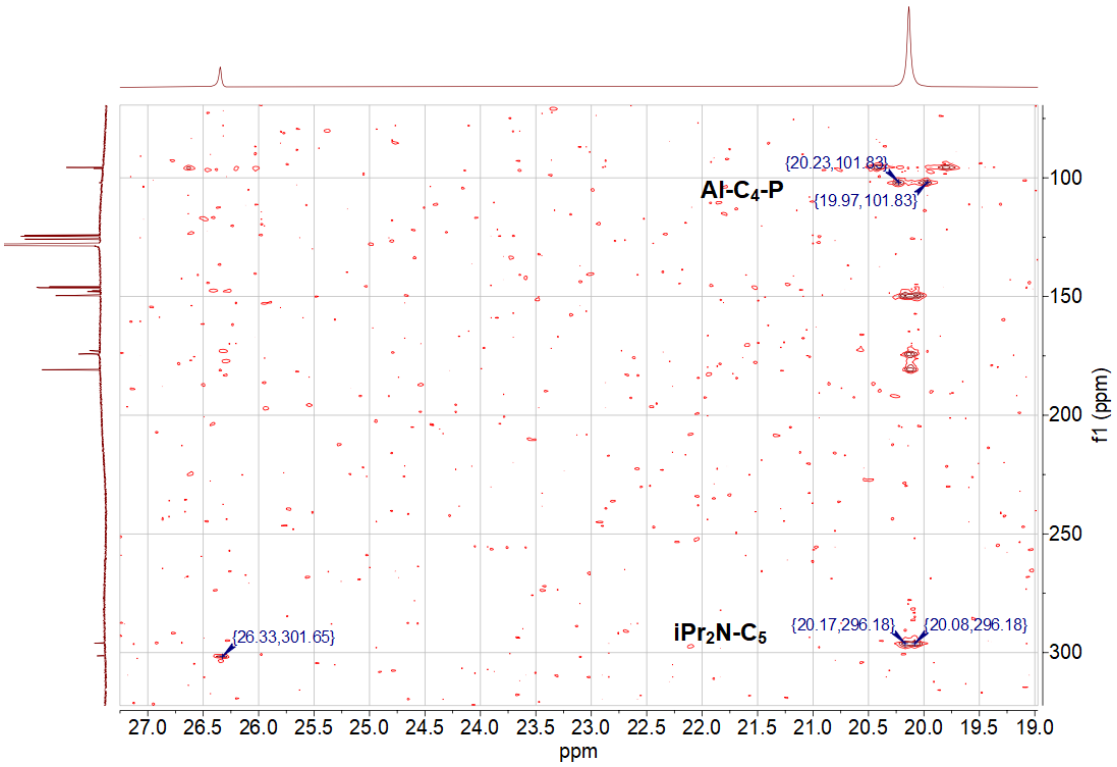
$^{13}C\{^{1}H\}$-NMR (upside) and $^{13}C\{^{1}H,^{31}P\}$-NMR (downside) (151 MHz, C_6D_6, 25 °C):



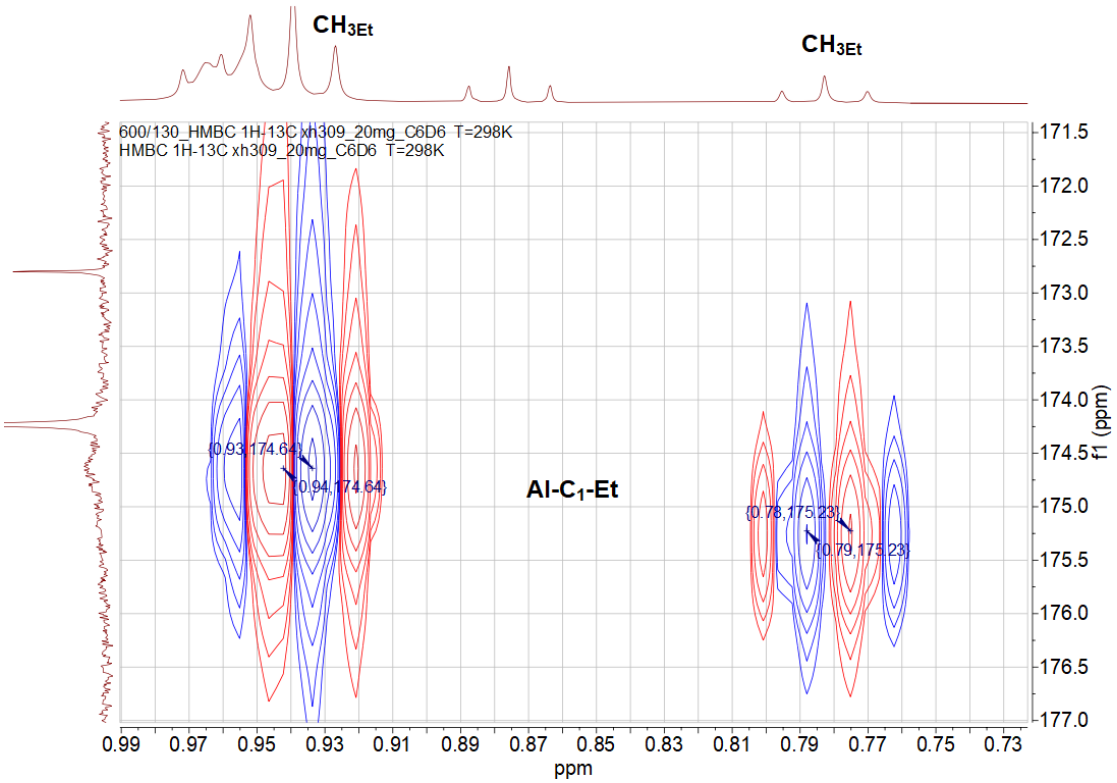
$^{13}C\{^{1}H\}$-NMR (upside) and $^{13}C\{^{1}H,^{31}P\}$-NMR (downside) (151 MHz, C_6D_6, 25 °C):



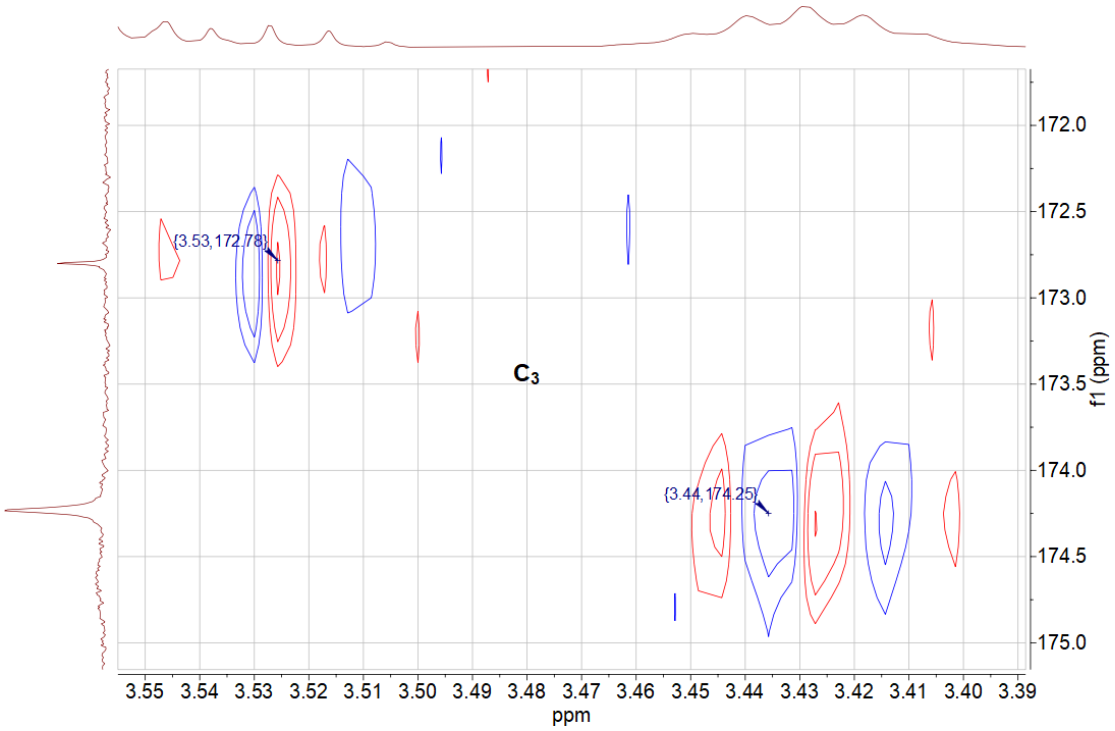
HMBC (^{31}P, ^{13}C) (C_6D_6, 25 °C):



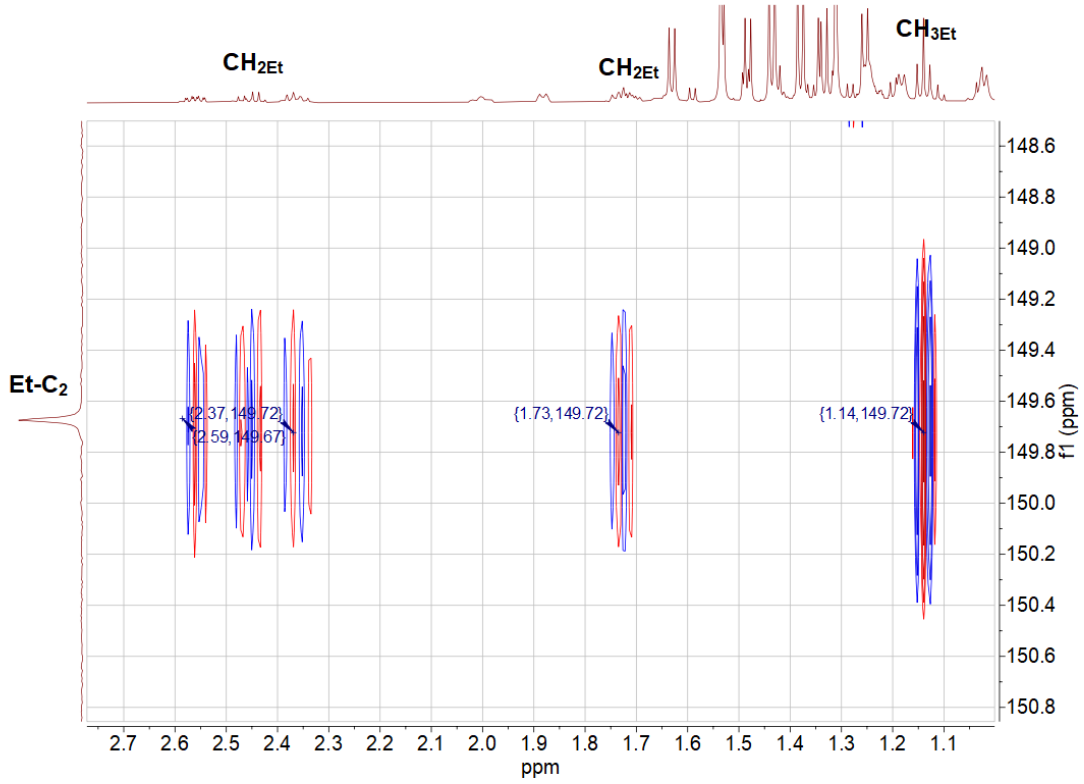
HMBC (^{1}H, ^{13}C) (C_6D_6, 25 °C):



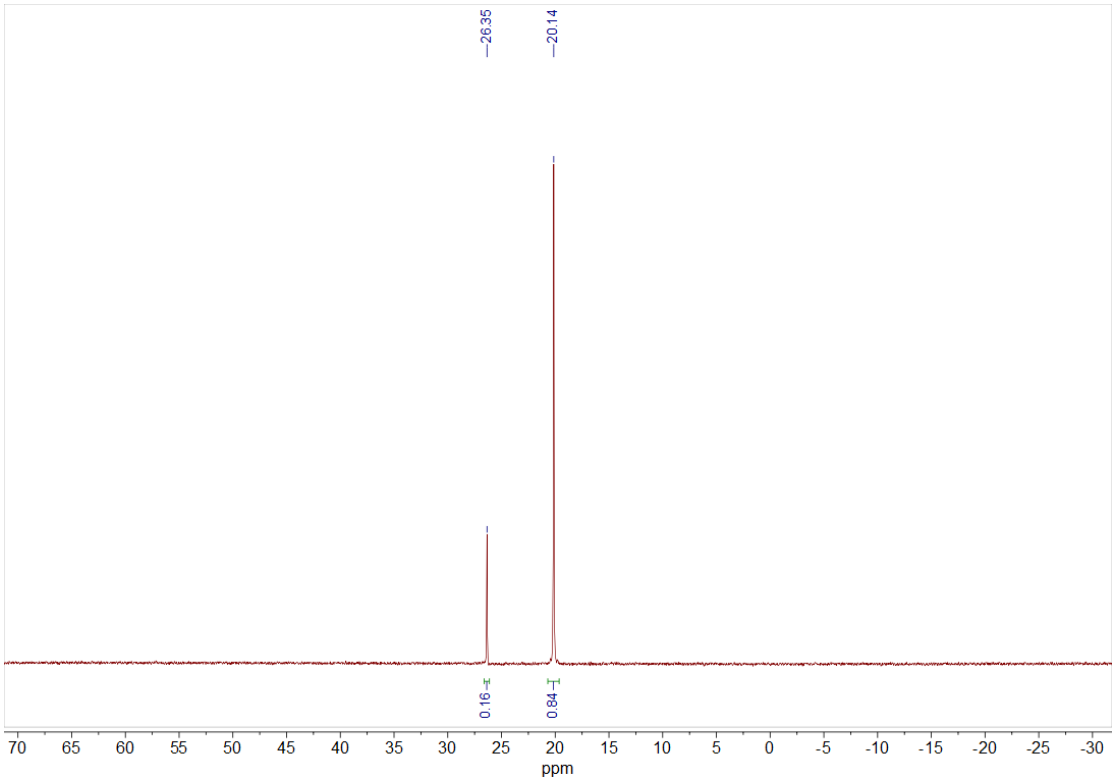
HMBC (^{1}H, ^{13}C) (C_6D_6, 25 °C):



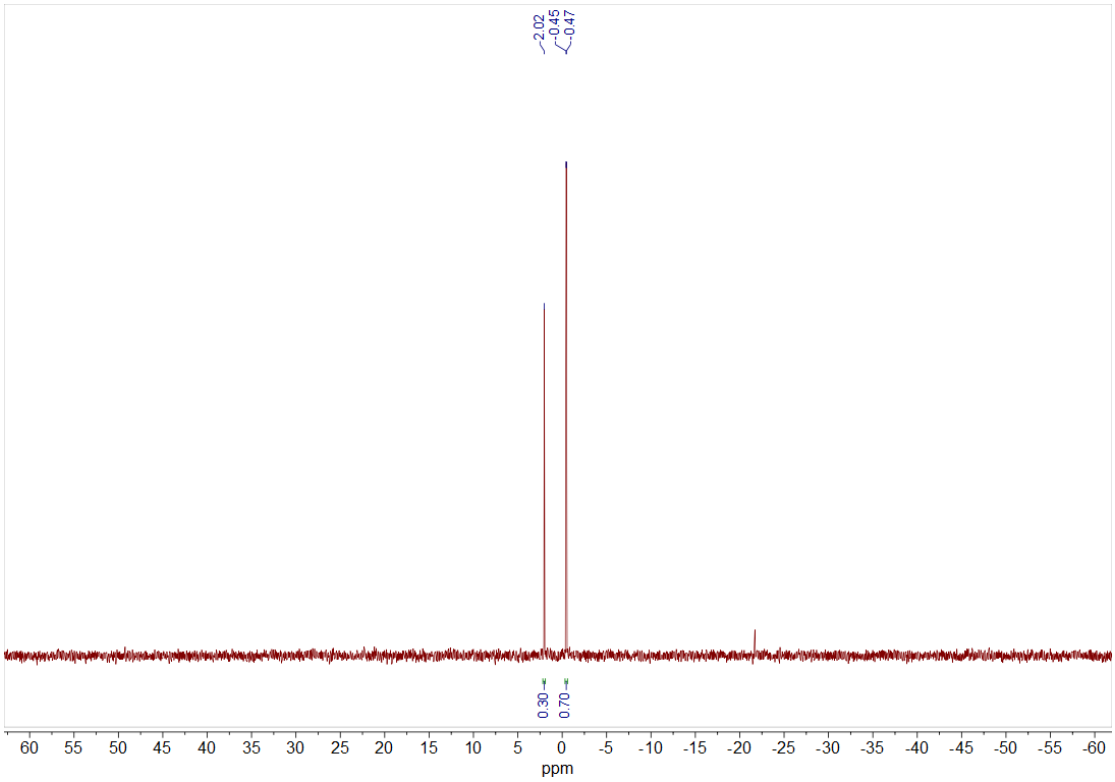
HMBC (^{1}H, ^{13}C) (C_6D_6, 25 °C):

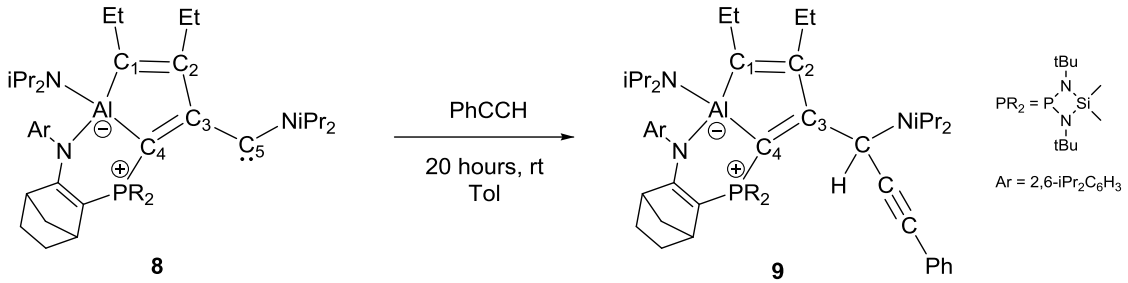


$^{31}P\{^{1}H\}$ NMR (243 MHz, C_6D_6, 25 °C):



$^{29}Si\{^{1}H\}$ NMR (79 MHz, C_6D_6, 25 °C):





Synthesis of 9: To a solution of **8** (200 mg, 0.214 mmol) in toluene (5.0 ml), phenylacetylene (24 μL, 0.214 mmol) was added at room temperature. After 20 hours at room temperature, all volatiles were removed under vacuum. The crude products were washed by acetonitrile (5ml X 3). After drying the solid under vacuum, **9** was obtained as pale brown powder (177 mg, yield = 80 %). Ratio major/minor isomers 3:1. Mp: 115 - 125 °C (decomp.).

Major diastereomer (75 %)

^{1}H NMR (400 MHz, THF-d_8, -40 °C): δ 0.29 (t, J_{HH} = 7.5 Hz, 3H, CH_{3Et}), 0.75 (s, 6H, $SiCH_3$), 0.86 (d, J_{HH} = 6.5 Hz, 3H, CH_{3iPr}), 0.90 (d, J_{HH} = 6.9 Hz, 3H, $CH_{3AlNiPr}$), 0.95 (t, J_{HH} = 6.9 Hz, 3H, CH_{3Et}), 1.00 (m, 3H, $CH_{3AlNiPr}$), 1.08 (d, J_{HH} = 6.5 Hz, 3H, CH_{3iPr}), 1.11 (d, J_{HH} = 6.5 Hz, 3H, $CH_{3AlNiPr}$), 1.14 (d, J_{HH} = 6.3 Hz, 6H, CH_{3NiPr}), 1.22 (d, J_{HH} = 6.5 Hz, 3H, CH_{3iPr}), 1.23 ($m_{overlapped}$, 1H, CH_2), 1.28 (br, 15H, $CH_{3AlNiPr}$ and CH_{3NiPr}), 1.31 ($m_{overlapped}$, 1H, CH_2), 1.36 (d, J_{HH} = 6.5 Hz, 3H, CH_{3iPr}), 1.47 (s, 9H, CH_{3tBu}), 1.59 (s, 9H, CH_{3tBu}), 1.61 ($m_{overlapped}$, 1H, CH_2), 1.69 (m, 1H, CH_{2Et}), 1.76 (m, 1H, CH_{2Et}), 1.89 (d, J_{PH} = 7.9 Hz, 1H, CH_2), 2.11 (m, 2H, CH_{2Et} and CH_2), 2.30 (m, 2H, CH_{2Et} and CH_2), 2.48 (s, 1H, $CH_{bridgehead}$), 2.89 (m, 1H, CH_{NiPr}), 3.10 (s, 1H, $CH_{bridgehead}$), 3.11 (m, 1H, CH_{iPr}), 3.47 (m, 3H, CH_{AlNiPr} and CH_{NiPr}), 4.41 (sept, J_{HH} = 6.7 Hz, 1H, CH_{iPr}), 5.20 (s, 1H, iPr_2N-CH), 6.95 – 7.08 (m, 2H, CH_{Ar}), 7.18 (m, 1H, CH_{Ar}), 7.28 – 7.45 (m, 5H, CH_{Ph}).

^{13}C{^{1}H} NMR (101 MHz, THF-d_8, -40 °C): δ 5.8 (s, $SiCH_3$), 6.7 (d, J_{CP} = 2.6 Hz, $SiCH_3$), 15.2 (s, CH_{3Et}), 16.3 (s, CH_{3Et}), 20.4 (s, $CH_{3AlNiPr}$ X 2), 23.1 (s, CH_{2Et}), 23.3 (s, CH_{3NiPr} X 2), 25.2 (s, $CH_{3AlNiPr}$ X 2), 25.2 (s, CH_{3NiPr} X 2), 25.8 (s, CH_2), 26.4 (s, CH_{AlNiPr} X 2), 26.7 (s, CH_{NiPr} X 2), 27.2 (s, CH_{2Et}), 27.5 (s, CH_{iPr} X 2), 28.2 (s, CH_{3iPr} X 2), 29.0 (s, CH_{3iPr} X 2), 30.4 (s, CH_2), 32.8 (d, J_{CP} = 4.0 Hz, CH_{3tBu}), 33.6 (d, J_{CP} = 4.4 Hz, CH_{3tBu}), 43.7 (d, J_{CP} = 14.3 Hz, $CH_{bridgehead}$), 47.2 (d, J_{CP} = 6.7 Hz, CH_2), 50.5 (d, J_{CP} = 12.3 Hz, $CH_{bridgehead}$), 53.0 (s, C_{tBu}), 53.9 (s, C_{tBu}), 56.3 (d, J_{CP} = 24.4 Hz, iPr_2N-CH), 88.7 (s, C≡C), 93.4 (d, J_{CP} = 2.37 Hz, C≡C), 98.8 (d, J_{CP} = 138.1 Hz, CP), 124.1 (s, CH_{Ar}), 125.0 (s, C_{Ph}), 125.2 (s, CH_{Ar}), 126.2 (s, CH_{Ar}), 129.0 (s, CH_{Ph}), 129.5 (s, CH_{Ph} x 2), 131.8 (s, CH_{Ph} x 2), 140.1 (d, J_{CP} = 36.9 Hz, Al-C_4-P), 145.5 (s, N-C_{Ar}), 145.9 (s, *i*Pr-C_{Ar}), 147.1 (s, *i*Pr-C_{Ar}), 153.5 (d, J_{CP} = 29.1 Hz, Et-C_2), 169.8 (d, J_{CP} = 12.5 Hz, C_3), 178.0 (br, Al-C_1-Et), 187.3 (d, J_{CP} = 7.9 Hz, NC).

^{31}P{^{1}H} NMR (162 MHz, THF-d_8, -40 °C): δ 32.2 (br, CP).

^{29}Si{^{1}H} NMR (80 MHz, THF-d_8, -40 °C): δ 8.2 (s, $SiCH_3$).

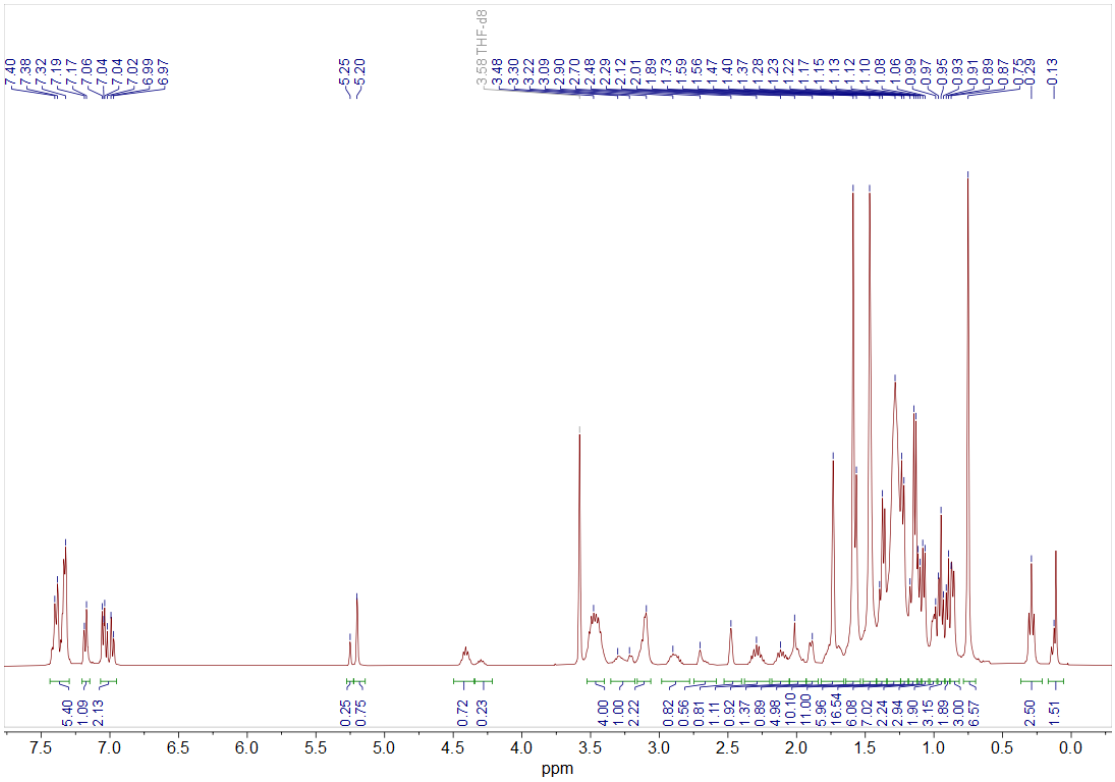
Minor diastereomer (25 %)

^{1}H NMR (400 MHz, THF-d_8, -40 °C): δ 0.13 (t, J_{HH} = 7.5 Hz, 3H, CH_{3Et}), 0.75 (s, 6H, $SiCH_3$), 0.95 ($t_{overlapped}$, 3H, CH_{3Et}),0.86 (d, J_{HH} = 6.5 Hz, 3H, CH_{3iPr}), 1.08 (d, J_{HH} = 6.5 Hz, 3H, CH_{3iPr}), 1.14 (m, 6H, $CH_{3AlNiPr}$), 1.15 ($d_{overlapped}$, 6H, CH_{3NiPr}), 1.23 ($d_{overlapped}$, 3H, CH_{3iPr}), 1.23 ($m_{overlapped}$, 1H, CH_2),

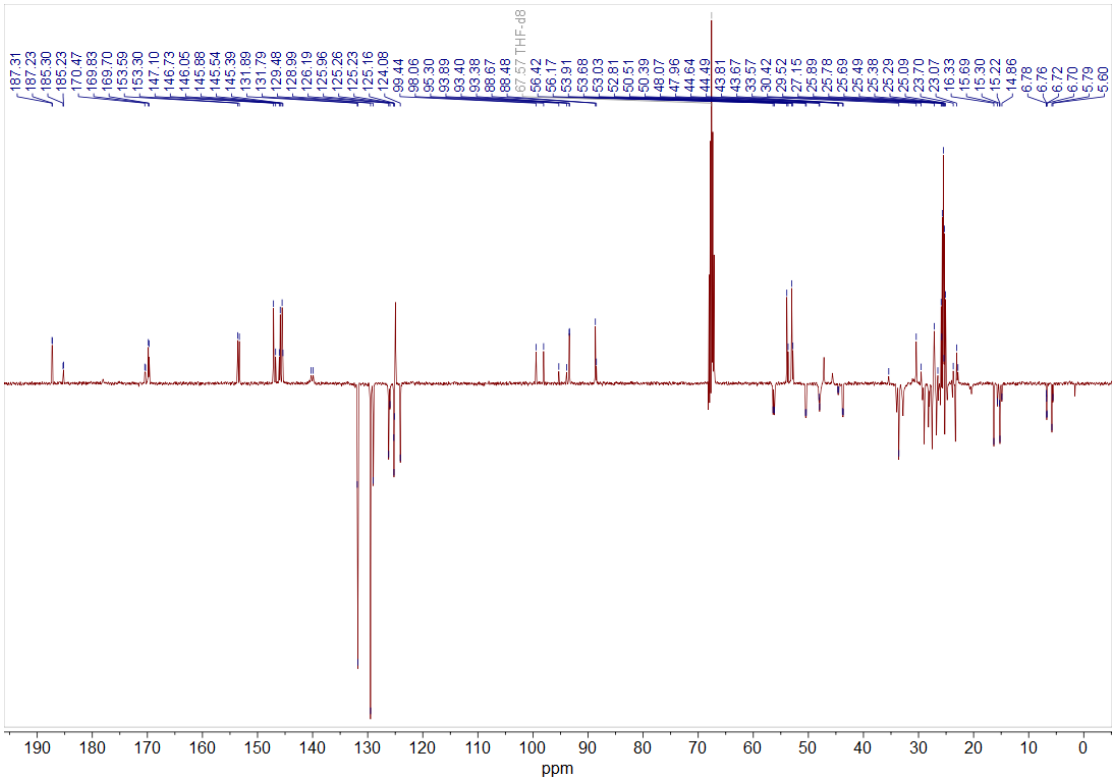
1.27 (br, 12H, $CH_{3AlNiPr}$ and CH_{3NiPr}), 1.39 ($d_{overlapped}$, 3H, CH_{3iPr}), 1.46 (s, 9H, CH_{3tBu}), 1.56 (s, 9H, CH_{3tBu}), 1.63 ($m_{overlapped}$, 1H, CH_2), 1.68 (m, 1H, CH_{2Et}), 1.70 ($m_{overlapped}$, 1H, CH_2), 1.76 (m, 1H, CH_{2Et}), 1.90 ($m_{overlapped}$, 1H, CH_2), 2.00 (m, 1H, CH_{2Et}), 2.30 (m, 1H, CH_{2Et}), 2.67 (m, 1H, CH_{NiPr}), 2.70 (s, 1H, $CH_{bridgehead}$), 3.21 (d, J_{HH} = 6.8 Hz, 1H, $CH_{bridgehead}$), 3.29 (m, 1H, CH_{iPr}), 3.48 (m, 3H, CH_{AlNiPr} and CH_{NiPr}), 4.30 (sept, J_{HH} = 6.7 Hz, 1H, CH_{iPr}), 5.25 (s, 1H, C_5H), 6.95 – 7.08 (m, 2H, CH_{Ar}), 7.18 (m, 1H, CH_{Ar}), 7.28–7.45 (m, 5H, CH_{Ph}).

$^{13}C\{^1H\}$ NMR (101 MHz, THF-d_8, -40 °C): δ 5.6 (s, $SiCH_3$), 6.8 (d, J_{CP} = 2.8 Hz, $SiCH_3$), 15.3 (s, CH_{3Et}), 15.7 (s, CH_{3Et}), 20.7 (s, $CH_{3AlNiPr}$ X 2), 22.8 (s, CH_{2Et}), 23.8 (s, CH_{3NiPr} X 2), 24.8 (s, $CH_{3AlNiPr}$ X 2) 25.2 (s, CH_{3NiPr} X 2), 25.8 (s, CH_2), 26.4 (s, CH_{AlNiPr} X 2), 26.5 (s, CH_{2Et}), 26.9 (s, CH_{NiPr} X 2), 27.6 (s, CH_{iPr} X 2), 28.0 (s, CH_{3iPr} X 2), 29.3 (s, CH_{3iPr} X 2), 29.5 (s, CH_2), 32.9 (d, J_{CP} = 3.5 Hz, CH_{3tBu}), 34.0 (d, J_{CP} = 4.8 Hz, CH_{3tBu}), 44.6 (d, J_{CP} = 15.4 Hz, $CH_{bridgehead}$), 45.6 (d, J_{CP} = 4.7 Hz, CH_2), 48.0 (d, J_{CP} = 11.6 Hz, $CH_{bridgehead}$), 52.8 (s, C_{tBu}), 53.7 (s, C_{tBu}), 56.3 (d, J_{CP} = 24.4 Hz, C_5H), 88.5 (s, C_7), 93.5 (d, J_{CP} = 2.3 Hz, C_6), 94.6 (d, J_{CP} = 141.7 Hz, CP), 125.0 (s, C_8), 125.2 (s, CH_{Ar}), 125.3 (s, CH_{Ar}), 126.0 (s, CH_{Ar}), 129.0 (s, CH_{Ph}), 129.5 (s, CH_{Ph}), 131.9 (s, CH_{Ph}), 140.3 (d, J_{CP} = 38.2 Hz, Al-C_4-P), 145.4 (s, N-C_{Ar}), 146.1 (s, iPr-C_{Ar}), 146.7 (s, iPr-C_{Ar}), 153.5 (d, J_{CP} = 29.1 Hz, Et-C_2), 170.4 (d, J_{CP} = 12.6 Hz, C_3), 175.0 (br, Al-C_1-Et), 185.3 (d, J_{CP} = 7.5 Hz, NC).
$^{31}P\{^1H\}$ NMR (162 MHz, THF-d_8, -40 °C): δ 30.4 (br, CP).
$^{29}Si\{^1H\}$ NMR (80 MHz, THF-d_8, -40 °C): δ 7.5 (s, $SiCH_3$).

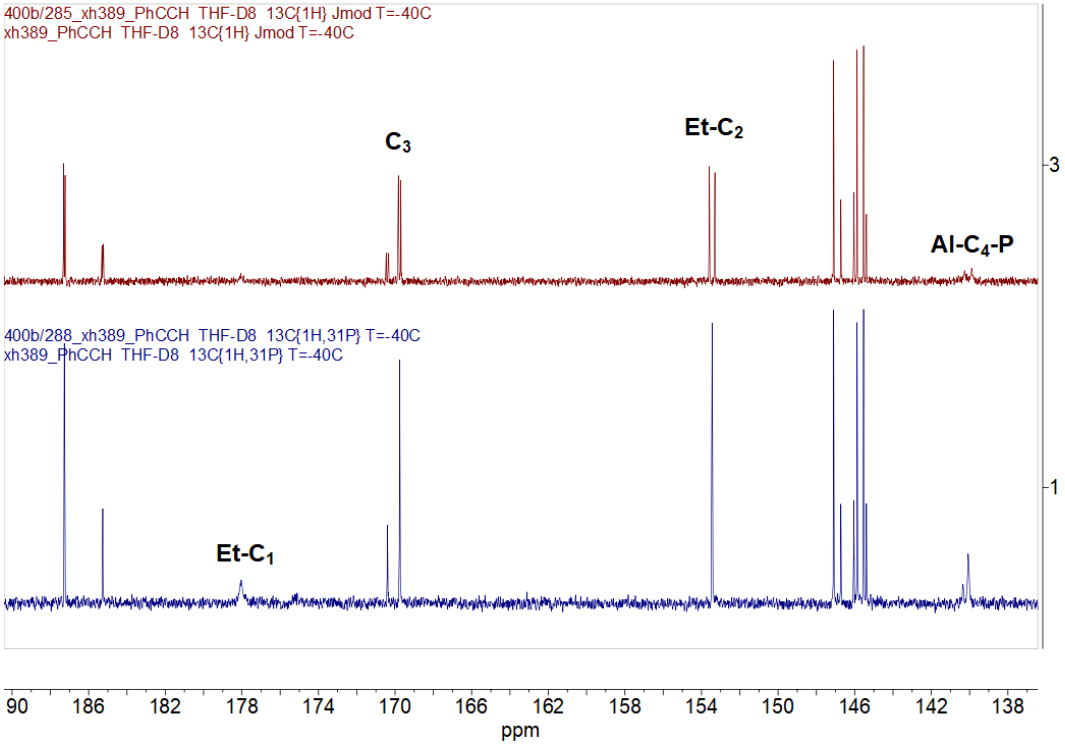
^{1}H NMR (400 MHz, THF-d_8, -40 °C):



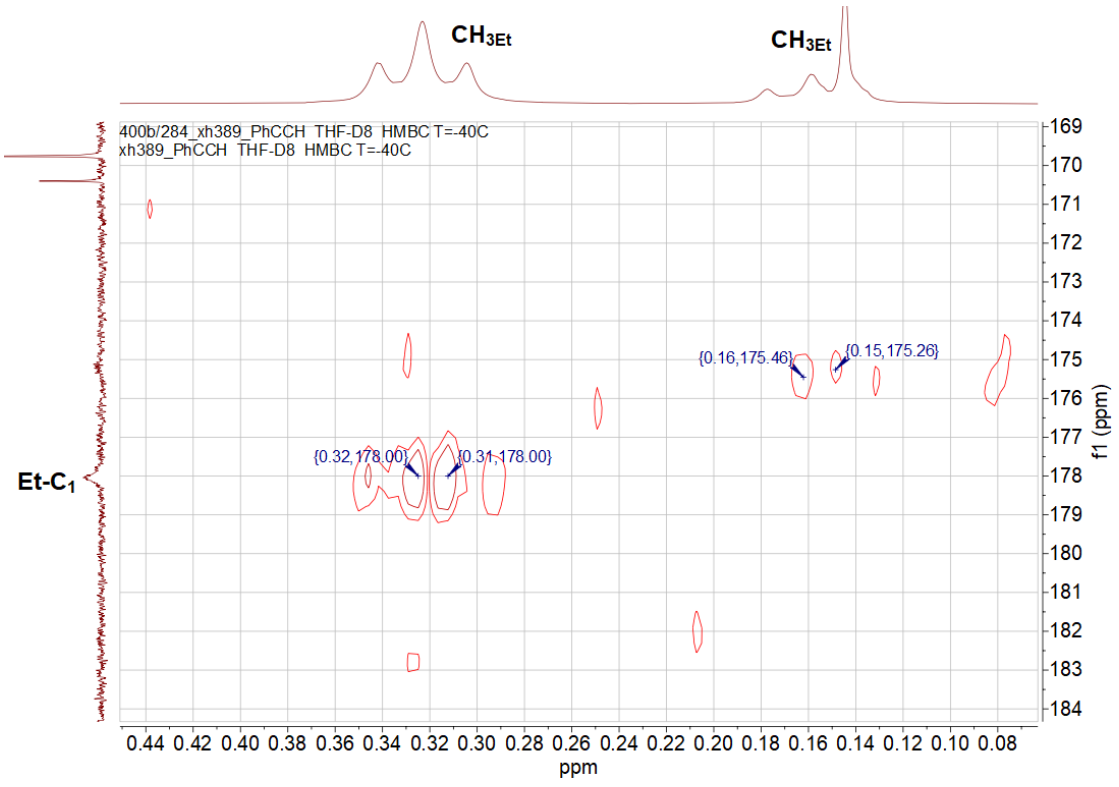
^{13}C{^{1}H} NMR (101 MHz, THF-d_8, -40 °C):



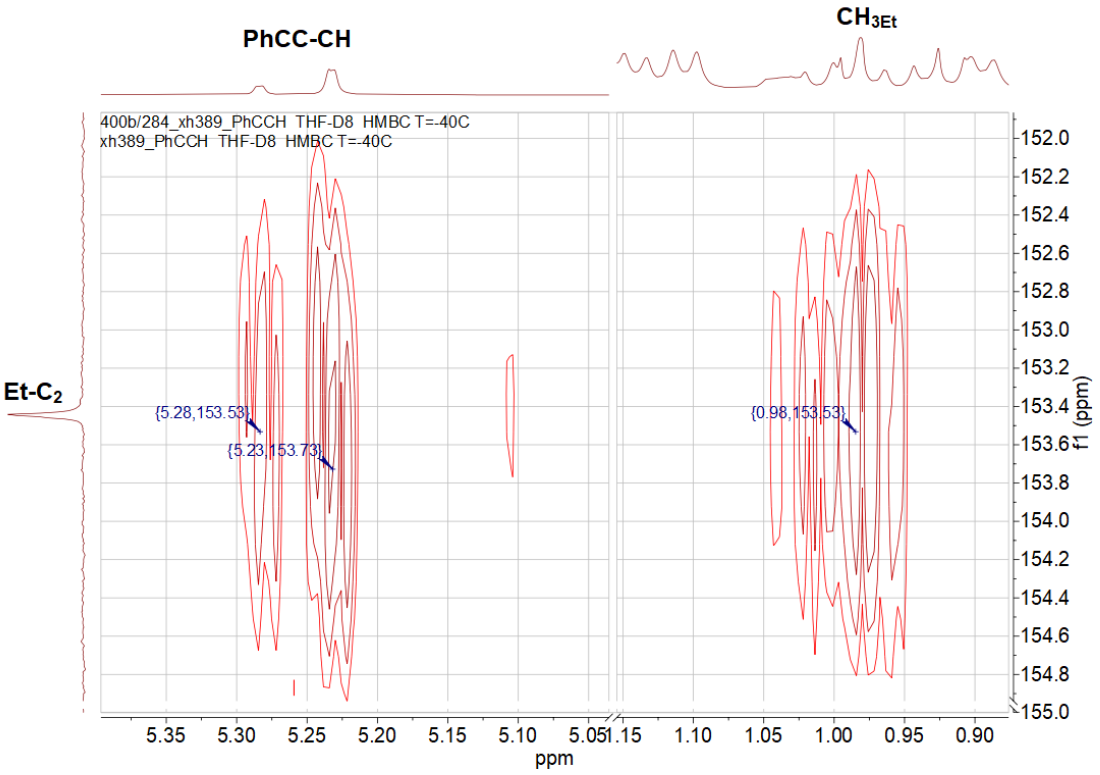
$^{13}C\{^{1}H\}$-NMR (upside) and $^{13}C\{^{1}H,^{31}P\}$-NMR (downside) (101 MHz, THF-d_8, -40 °C):



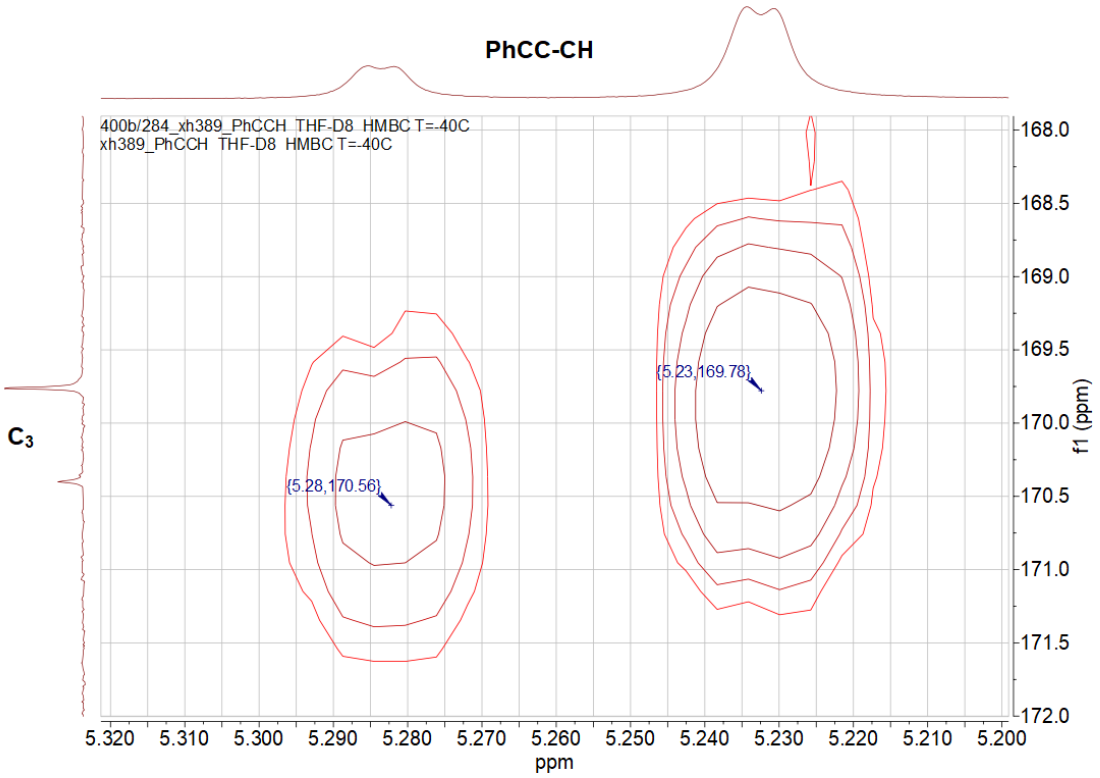
HMBC (^{1}H, ^{13}C) (THF-d_8, -40 °C):



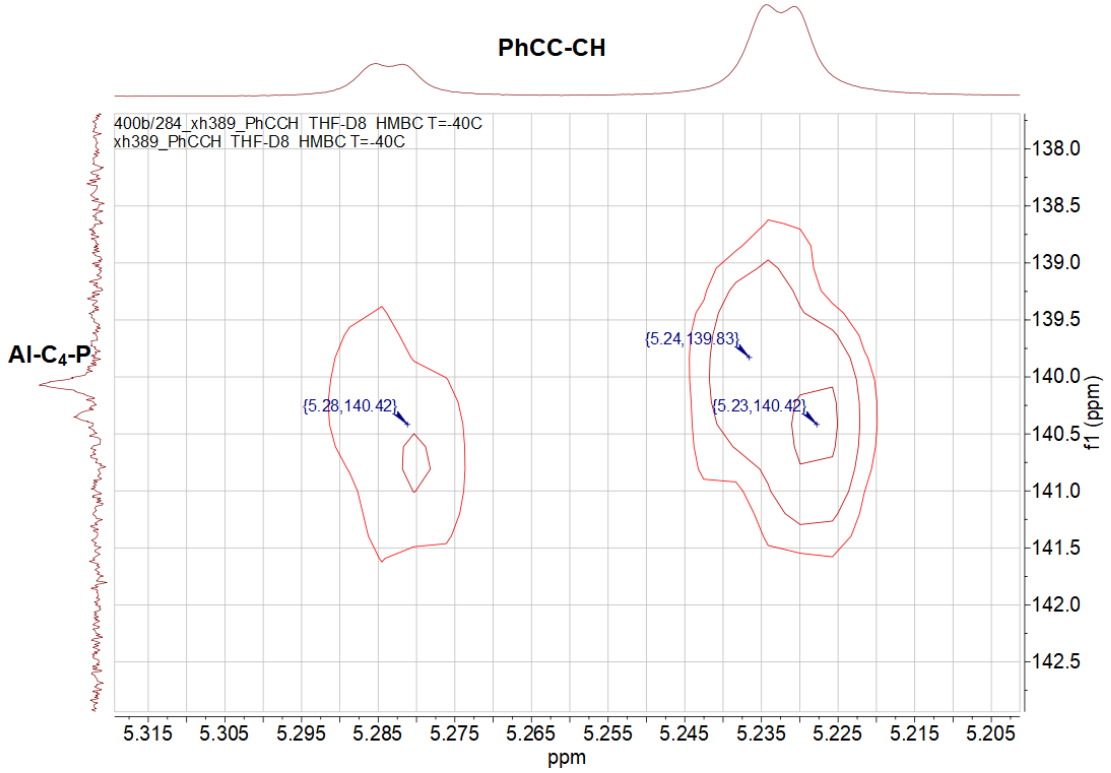
HMBC (^{1}H, ^{13}C) (THF-d_8, -40 °C):



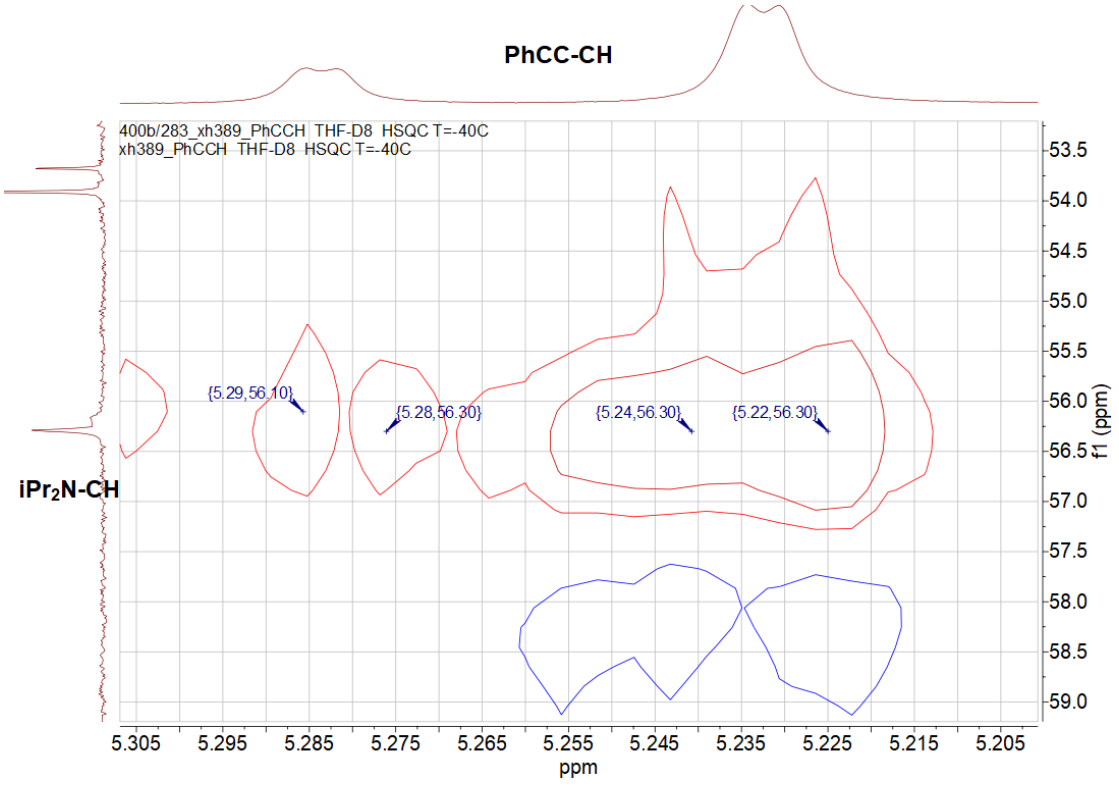
HMBC (^{1}H, ^{13}C) (THF-d_8, -40 °C):



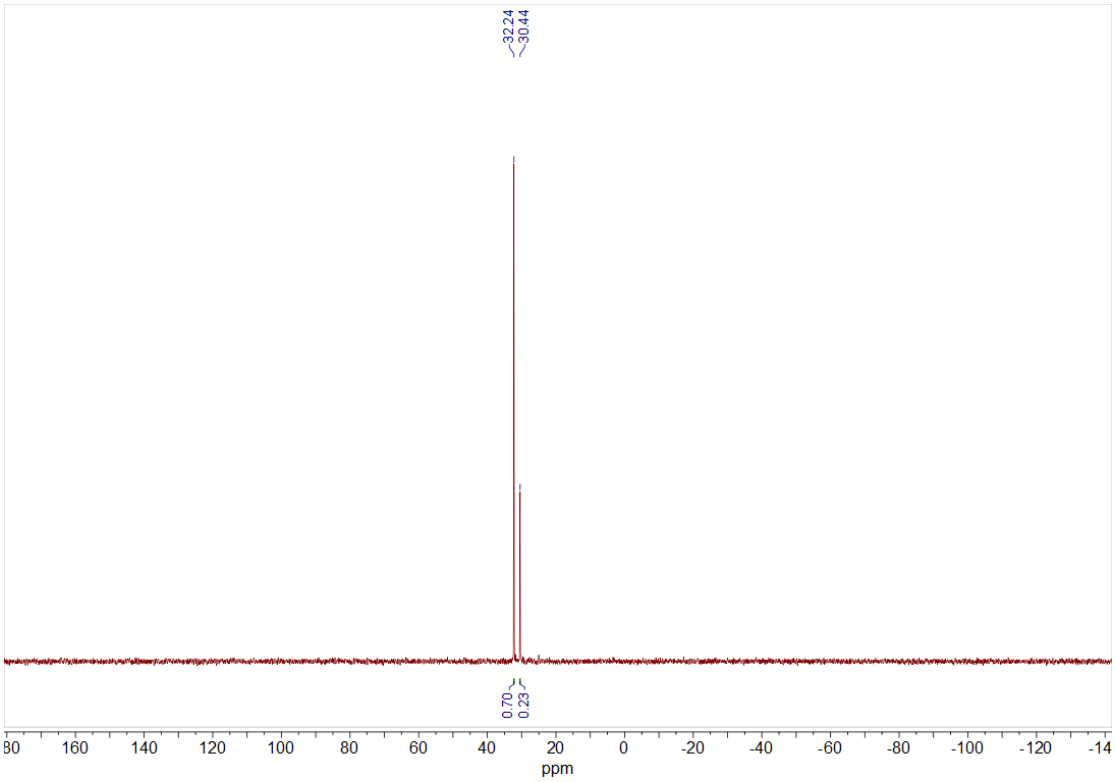
HMBC (^{1}H, ^{13}C) (THF-d_8, -40 °C):



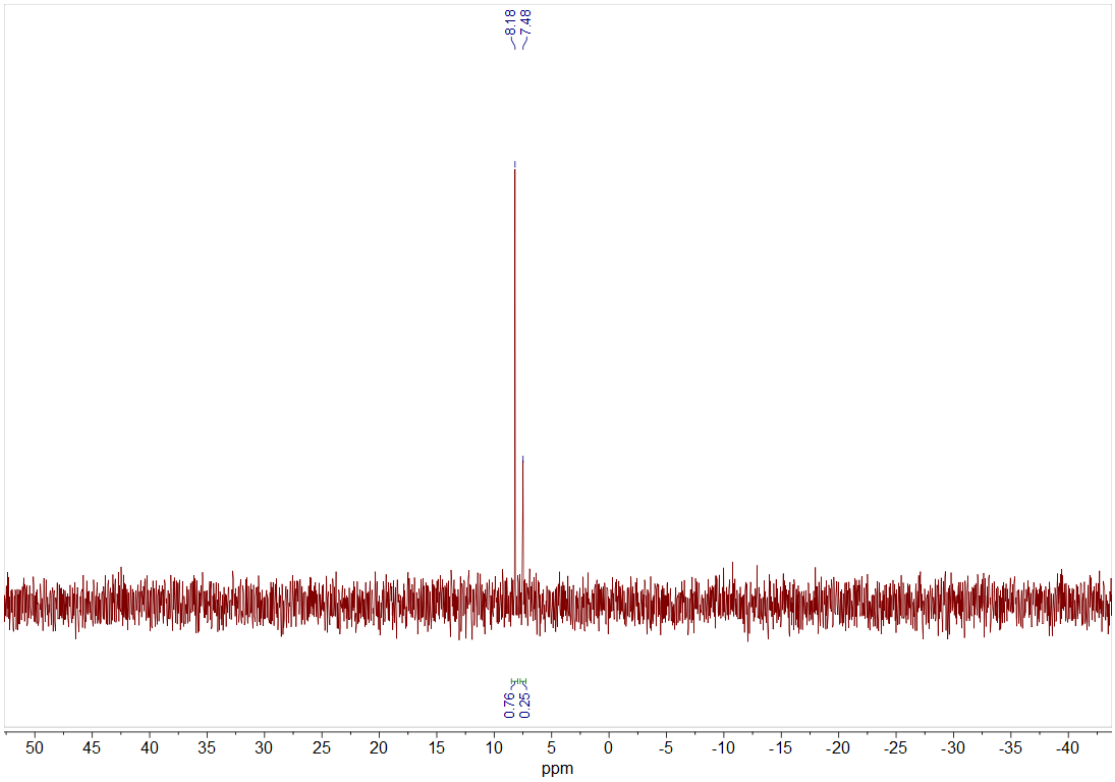
HSQC (^{1}H, ^{13}C) (THF-d_8, -40 °C):

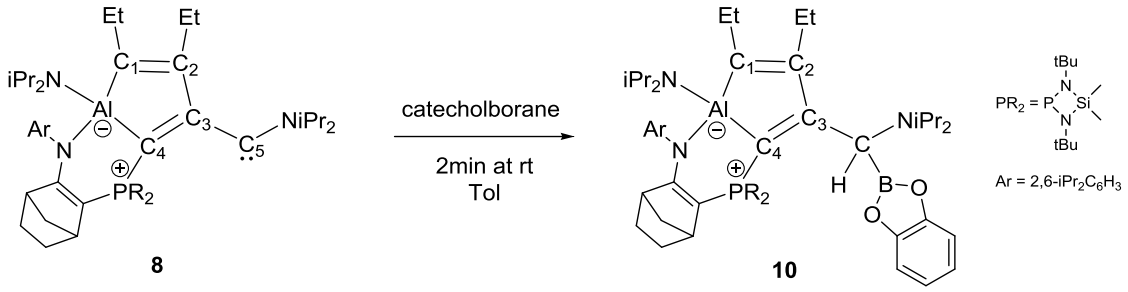


$^{31}P\{^{1}H\}$ NMR (162 MHz, THF-d_8, -40 °C):



$^{29}Si\{^{1}H\}$ NMR (80 MHz, THF-d_8, -40 °C):





8 10

Synthesis of 10: To a solution of **8** (200 mg, 0.214 mmol) in toluene (5.0 ml), catecholborane (23 μL, 0.214 mmol, 1 eqv.) was added at room temperature. After 5 min at room temperature, all volatiles were removed under vacuum. The crude products were washed by acenitrile (5ml X 3). The resulting solid was dried under vacuum to obtain **10** as a yellow powder (155 mg, yield = 69 %). Ratio major/minor isomers 80:20. Mp: 125-135 °C (decomp.).

Major diastereomer (80 %)

^{1}H NMR (600 MHz, THF-d_8, -40 °C): δ 0.42 (t, J_{HH} = 7.5 Hz, 3H, CH_{3Et}), 0.69 (s, 3H, $SiCH_3$), 0.72 (s, 3H, $SiCH_3$), 0.99 (t, J_{HH} = 7.1 Hz, 3H, CH_{3Et}), 1.12 (m, 9H, $CH_{3AlN\mathit{i}Pr}$), 1.14 (s, 9H, $CH_{3\mathit{t}Bu}$), 1.18 (d, J_{HH} = 6.5 Hz, 6H, $CH_{3\mathit{i}Pr}$), 1.19 (m, 1H, CH_2), 1.23 (m, 1H, CH_2), 1.24 (d , J_{HH} = 6.6 Hz, 3H, $CH_{3AlN\mathit{i}Pr}$), 1.30 (d , J_{HH} = 6.5 Hz, 6H, $CH_{3N\mathit{i}Pr}$), 1.36 (m, 1H, CH_2), 1.38 (m, 6H, $CH_{3N\mathit{i}Pr}$), 1.40 (m, 6H, $CH_{3\mathit{i}Pr}$), 1.48 (s, 9H, $CH_{3\mathit{t}Bu}$), 1.58 (m, 1H, CH_2), 1.69 (m, 1H, CH_2), 1.90 (m, 1H, CH_2), 1.98 (m, 2H, CH_{2Et}), 2.19 (m, 2H, CH_{2Et}), 2.51 (s, 1H, $CH_{bridgehead}$), 3.08 (s, 1H, $CH_{bridgehead}$), 3.23 (m, 1H, $CH_{\mathit{i}Pr}$), 3.55 (m, 2H, $CH_{AlN\mathit{i}Pr}$), 3.73 (m, 2H, $CH_{N\mathit{i}Pr}$), 4.50 (m, 1H, $CH_{\mathit{i}Pr}$), 4.53 (s, 1H, BCH), 7.08 (m, 2H, CH_{Ar}), 7.13 (m, 2H, CH_{ph}), 7.21 (m, 1H, CH_{Ar}), 7.25 (m, 2H, CH_{ph}).

^{13}C{^{1}H} NMR (151 MHz, THF-d_8, -40 °C): δ 5.6 (s, $SiCH_3$), 6.8 (d, J_{CP} = 2.8 Hz, $SiCH_3$), 14.5 (s, CH_{3Et}), 17.4 (s, CH_{3Et}), 23.4 (br, $CH_{3N\mathit{i}Pr}$ X 2), 23.7 (s, $CH_{3\mathit{i}Pr}$ X 2), 25.2 (br, $CH_{3AlNiPr}$ X 2), 25.9 (s, CH_{2Et}), 26.0 (br, $CH_{3N\mathit{i}Pr}$ X 2), 26.9 (s, CH_{3iPr} X 2), 27.5 (s, $CH_{3AlNiPr}$ X 2), 27.6 (s, CH_2), 28.2 (s, $CH_{\mathit{i}Pr}$), 28.9 (s, CH_{iPr}), 29.2 (br, CH_2), 30.2 (s, CH_{2Et}), 32.4 (d, J_{CP} = 4.1 Hz, CH_{3tBu}), 33.5 (d, J_{CP} = 4.6 Hz, CH_{3tBu}), 43.9 (d, J_{CP} = 14.4 Hz, $CH_{bridgehead}$), 46.9 (d, J_{CP} = 6.7 Hz, CH_2), 48.3 (br, CH_{AlNiPr} X 2), 50.2 (d, J_{CP} = 12.2 Hz, $CH_{bridgehead}$), 52.5 (br, CH_{NiPr} X 2), 53.0 (s, C_{tBu}), 53.0 (s, C_{tBu}), 58.7 (br, BCH), 97.6 (d, J_{CP} = 139.0 Hz, CP), 113.3 (s, CH_{Ph} X 2), 123.9 (s, CH_{Ph} X 2), 124.0 (s, CH_{Ar}), 125.2 (s, CH_{Ar}), 126.3(s, CH_{Ar}), 138.1 (d, J_{CP} = 38.2 Hz, Al-C_4-P), 145.7 (s, N-C_{Ar}), 146.2 (s, iPr-C_{Ar}), 147.2(s, iPr-C_{Ar}), 148.6 (s, C_{Ph} X 2), 153.6 (d, J_{CP} = 30.8 Hz, Et-C_2), 175.4 (d, J_{CP} = 11.5 Hz, C_3), 176.1 (br, Al-C_1-Et), 187.2 (d, J_{CP} = 7.9 Hz, NC).

^{31}P{^{1}H} NMR (162 MHz, THF-d_8, -40 °C): δ 32.4 (s, CP).

^{29}Si{^{1}H} NMR (80 MHz, THF-d_8, -40 °C): δ 7.6 (s, $SiCH_3$).

^{11}B{^{1}H} NMR (128 MHz, THF-d_8, -40 °C): δ 33.7 (br, Bcat).

Minor diastereomer (20 %)

^{1}H NMR (600 MHz, THF-d_8, -40 °C): δ 0.20 (t, J_{HH} = 7.6 Hz, 3H, CH_{3Et}), 0.71 (s, 3H, $SiCH_3$), 0.77 (s, 3H, $SiCH_3$), 0.89 (m, 3H, $CH_{3\mathit{i}Pr}$), 0.99 (t, J_{HH} = 7.0 Hz, 3H, CH_{3Et}), 1.04 (m, 3H, $CH_{3\mathit{i}Pr}$), 1.09 (m, 1H, CH_2), 1.11 (m, 9H, $CH_{3AlN\mathit{i}Pr}$), 1.14 (s, 9H, $CH_{3\mathit{t}Bu}$), 1.20 (m, 6H, $CH_{3\mathit{i}Pr}$), 1.24 (m, 3H, $CH_{3AlN\mathit{i}Pr}$), 1.28 (m, 6H, CH_{3NiPr}), 1.38 (m, 6H, $CH_{3N\mathit{i}Pr}$), 1.44 (m, 6H, $CH_{3\mathit{i}Pr}$), 1.45 (m, 1H, CH_2), 1.47 (s, 9H, $CH_{3\mathit{t}Bu}$), 1.51 (m, 1H, CH_2), 1.67 (m, 1H, CH_2), 2.21 (m, 2H, CH_{2Et}), 2.41 (m, 2H, CH_{2Et}), 2.65 (s, 1H, $CH_{bridgehead}$), 3.11 (s, 1H, $CH_{bridgehead}$), 3.23 (m, 1H, $CH_{\mathit{i}Pr}$), 3.45 (m, 2H, $CH_{N\mathit{i}Pr}$), 3.60 (m, 2H,

CH_{AlNiPr}), 4.28 (m, 1H, CH_{iPr}), 4.74 (s, 1H, C_5H), 7.08 (m, 2H, CH_{Ar}), 7.13 (m, 2H, CH_{ph}), 7.21 (m, 1H, CH_{Ar}), 7.25 (m, 2H, CH_{ph}).

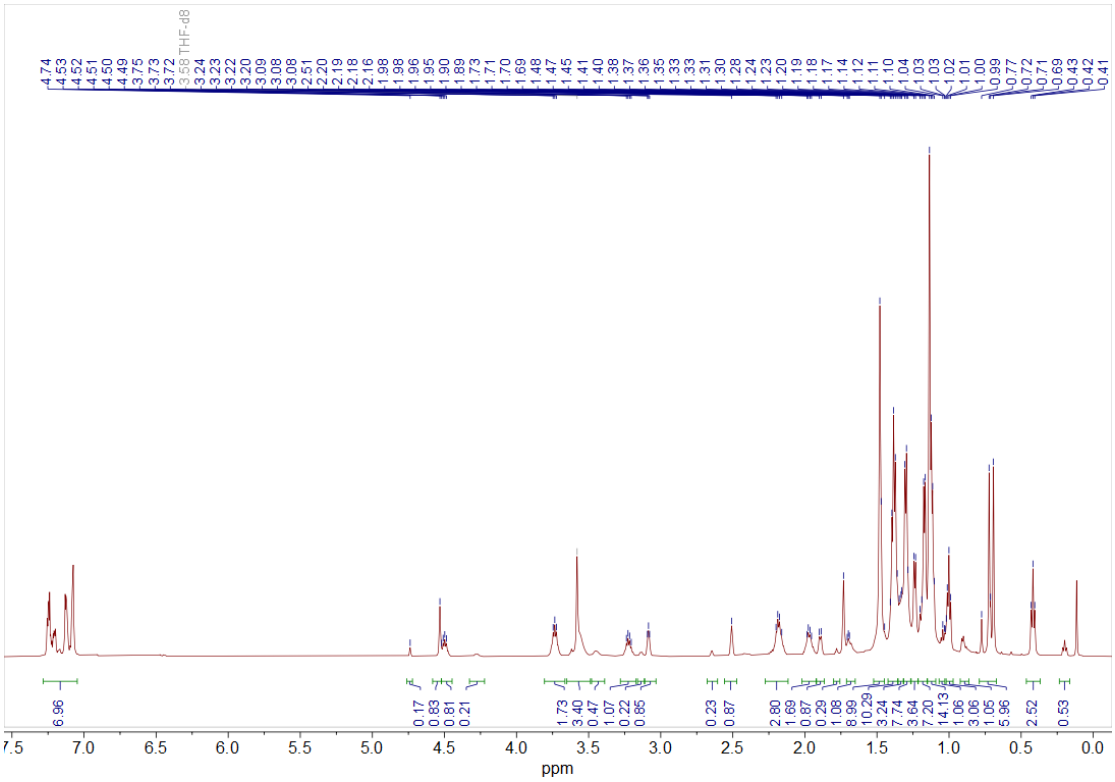
$^{13}C\{^1H\}$ NMR (151 MHz, THF-d_8, -40 °C): δ 5.3 (s, $SiCH_3$), 7.0 (d, J_{cp} = 2.8 Hz, $SiCH_3$), 14.6 (s, CH_{3Et}), 16.1 (s, CH_{3Et}), 24.1 (br, CH_{3NiPr} X 2), 25.1 (s, CH_2), 25.2 (s, $CH_{3AlNiPr}$ X 2), 26.4 (br, CH_{3NiPr} X 2), 26.8 (s, CH_2), 27.1 (s, CH_{3iPr} X 2),27.6 (s, $CH_{3AlNiPr}$ X2), 27.7 (s, CH_2), 28.0 (s, CH_{iPr} X 2), 29.4 (s, CH_{2Et}), 32.2 (d, J_{CP} = 4.4 Hz, CH_{3tBu}), 34.1 (d, J_{CP} = 4.5 Hz, CH_{3tBu}), 44.8 (d, J_{CP} = 15.2 Hz, $CH_{bridgehead}$), 46.2 (d, J_{CP} = 4.4 Hz, CH_2), 47.9 (d, J_{CP} = 11.6 Hz, $CH_{bridgehead}$), 52.7 (s, C_{tBu}), 52.9 (s, C_{tBu}), 54.4 (br, detected by HMBC(13C-31P), CH_{NiPr} X 2), 59.6 (br, BCH), 94.4 (d, J_{CP} = 140.2 Hz, CP), 113.4 (s, CH_{Ph} X 2), 124.0 (s, CH_{Ph} X 2), 125.1 (s, CH_{Ar} X 2), 126.0(s, CH_{Ar}), 138.1 (d, J_{CP} = 38.2 Hz, Al-C_4-P), 145.6 (s, N-C_{Ar}), 146.2 (s, iPr-C_{Ar}), 147.1 (s, iPr-C_{Ar}), 148.6 (s, OC X 2), 154.5 (d, J_{CP} = 30.1 Hz, Et-C_2), 174.8 (br, Al-C_1-Et), 175.5 (d, J_{CP} = 11.6 Hz, C_3), 185.0 (d, J_{CP} = 7.8 Hz, NC).

$^{31}P\{^1H\}$ NMR (162 MHz, THF-d_8, -40 °C): δ 32.0 (s, CP).

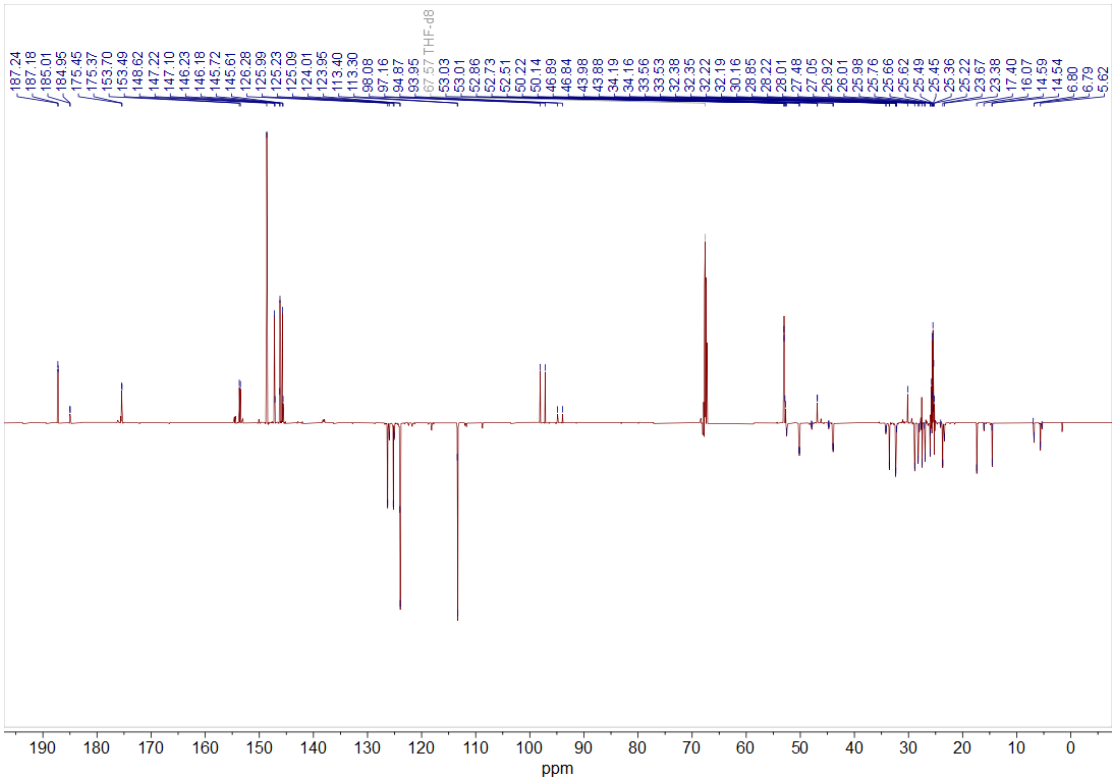
$^{29}Si\{^1H\}$ NMR (80 MHz, THF-d_8, -40 °C): δ 6.9 (s, $SiCH_3$).

$^{11}B\{^1H\}$ NMR (128 MHz, THF-d_8, -40 °C): δ 33.7 (br, Bcat).

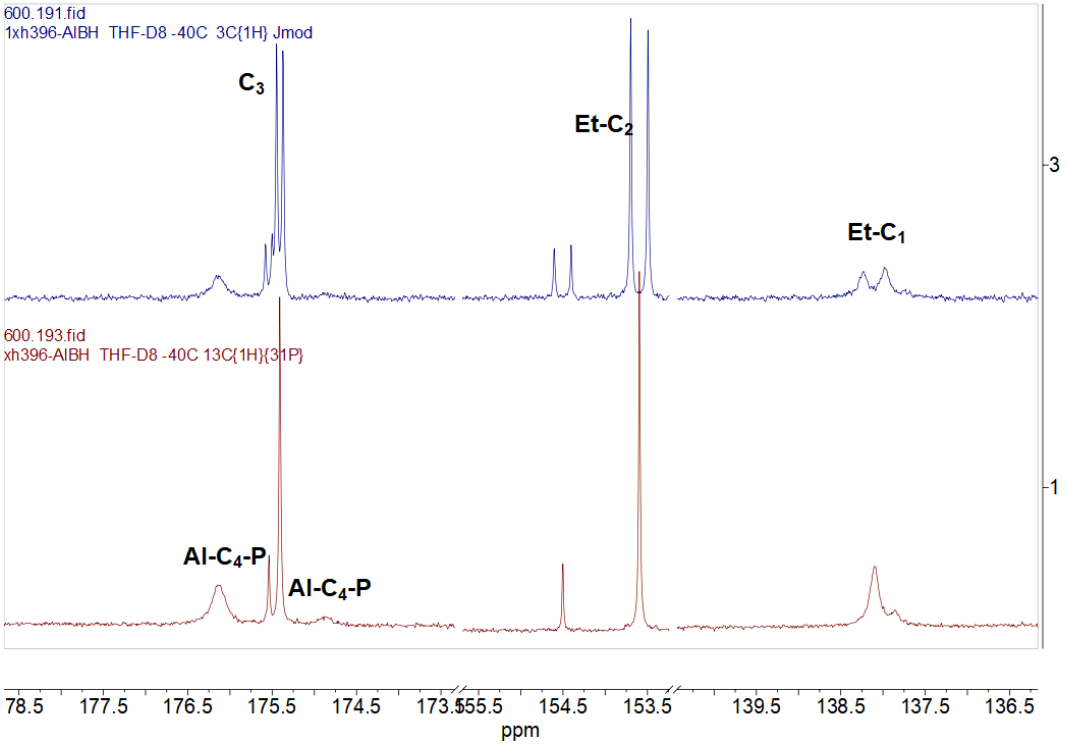
^{1}H NMR (600 MHz, THF-d_8, -40 °C):



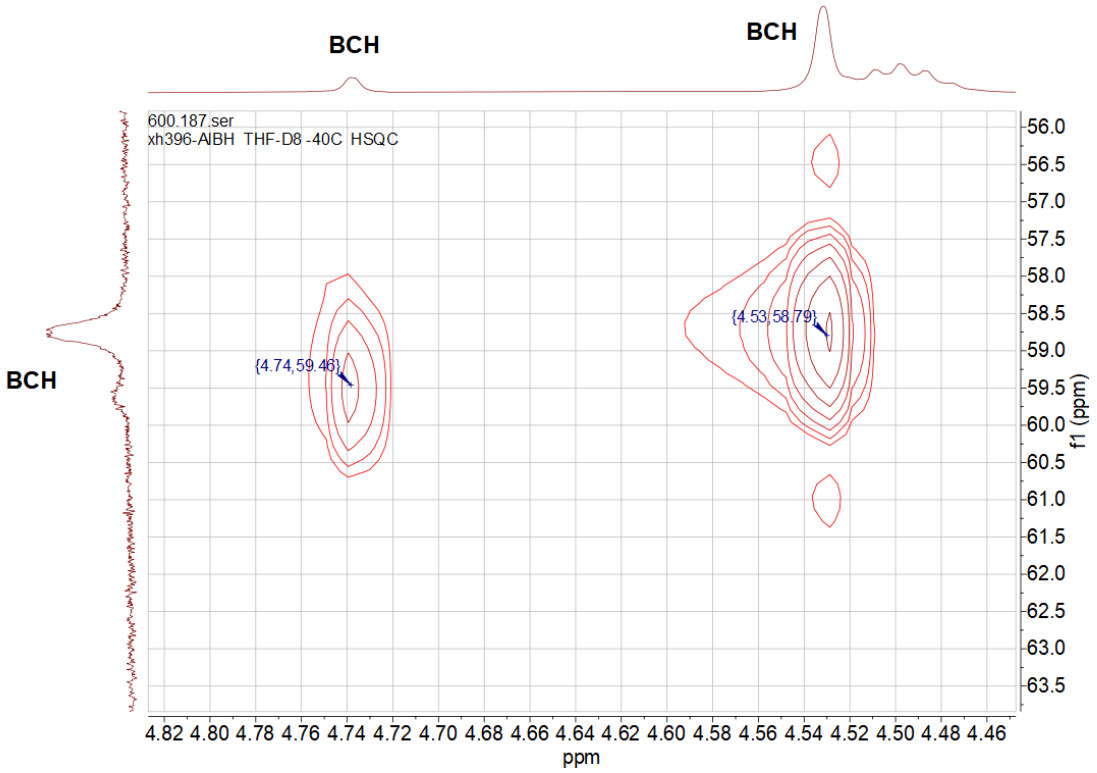
^{13}C{^{1}H} NMR (151 MHz, THF-d_8, -40 °C):



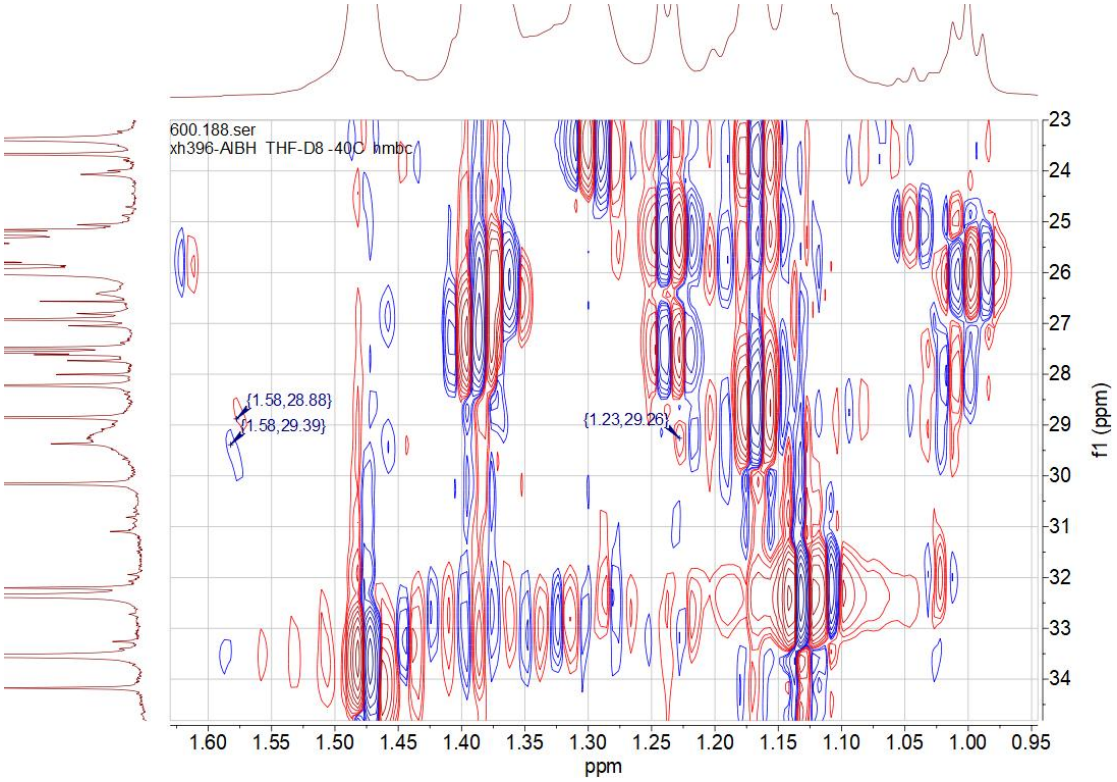
$^{13}C\{^{1}H\}$-NMR (upside) and $^{13}C\{^{1}H,^{31}P\}$-NMR (downside) (151 MHz, THF-d_8, -40 °C):



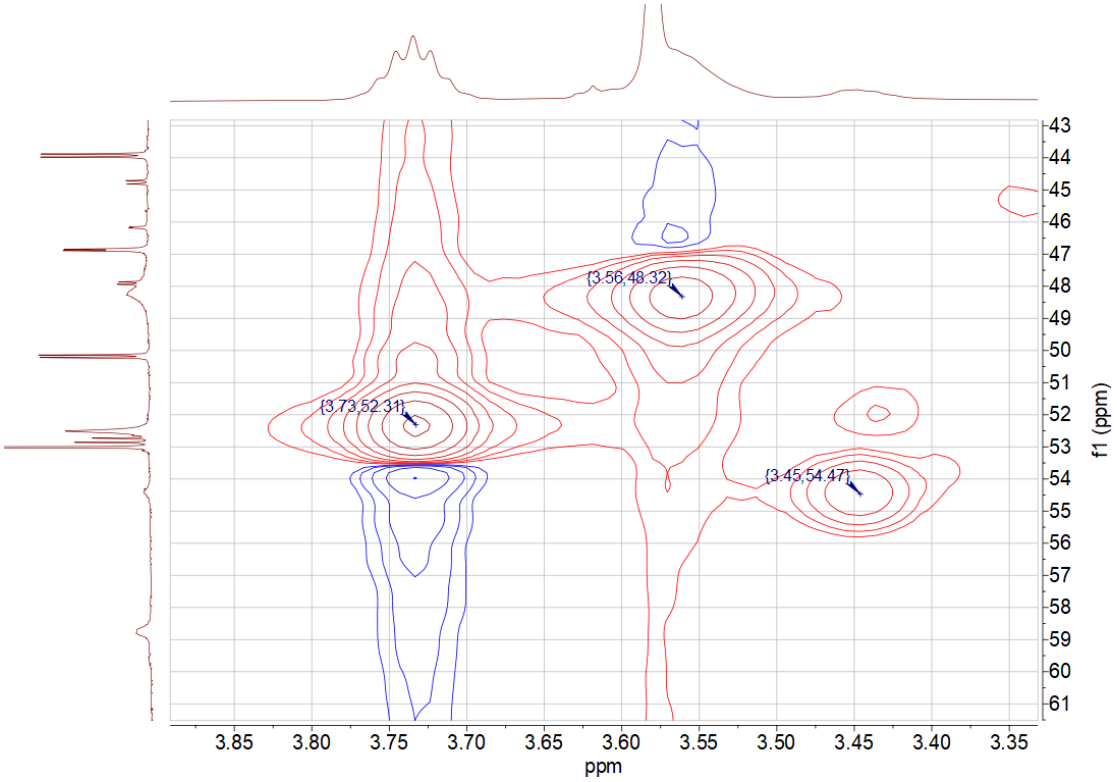
HSQC (^{1}H, ^{13}C) (THF-d_8, -40 °C) for ^{13}C NMR of BCH (δ 58.7; δ 59.6):



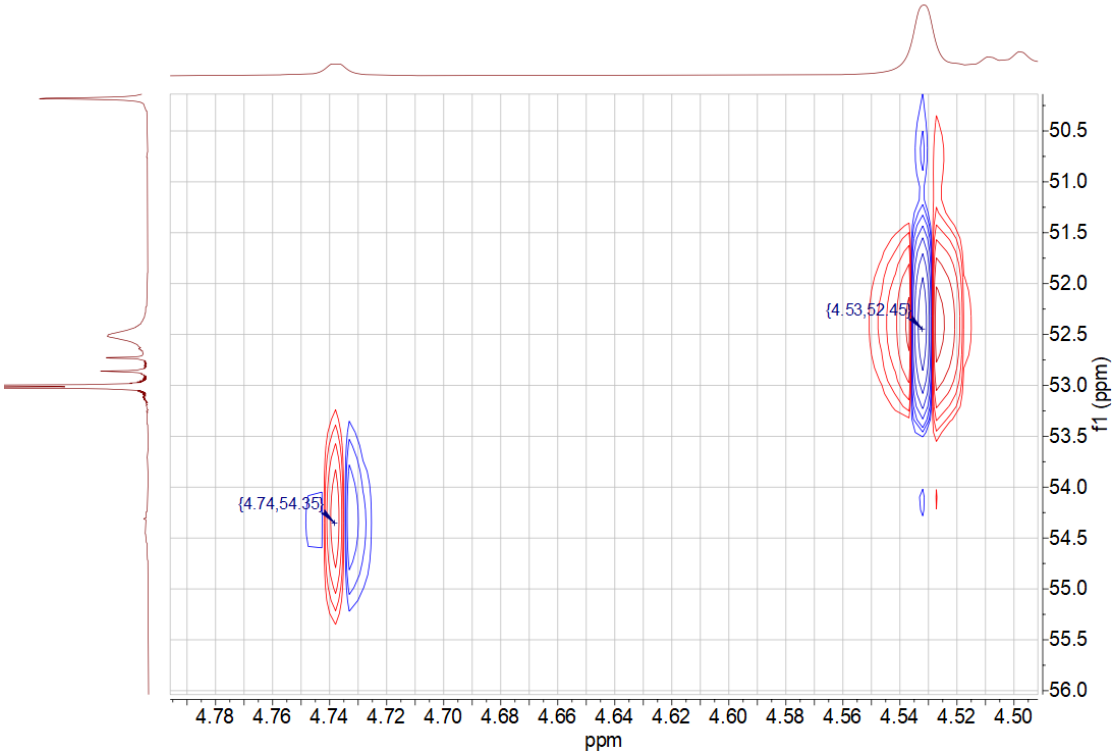
HMBC (^{1}H, ^{13}C) (THF-d_8, -40 °C) for ^{13}C NMR of CH_2 (δ 29.2):



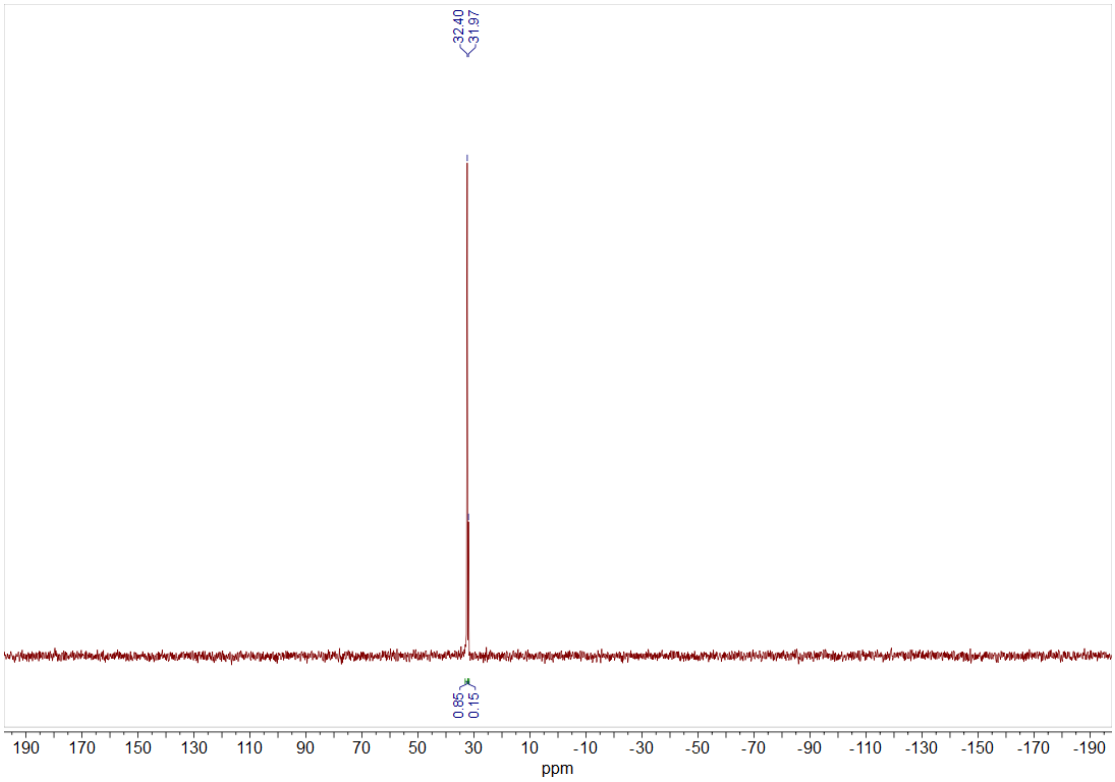
HSQC (^{1}H, ^{13}C) (THF-d_8, -40 °C) for ^{13}C NMR of CH_{AlNiPr} (δ 48.3) and CH_{NiPr} (δ 52.5):



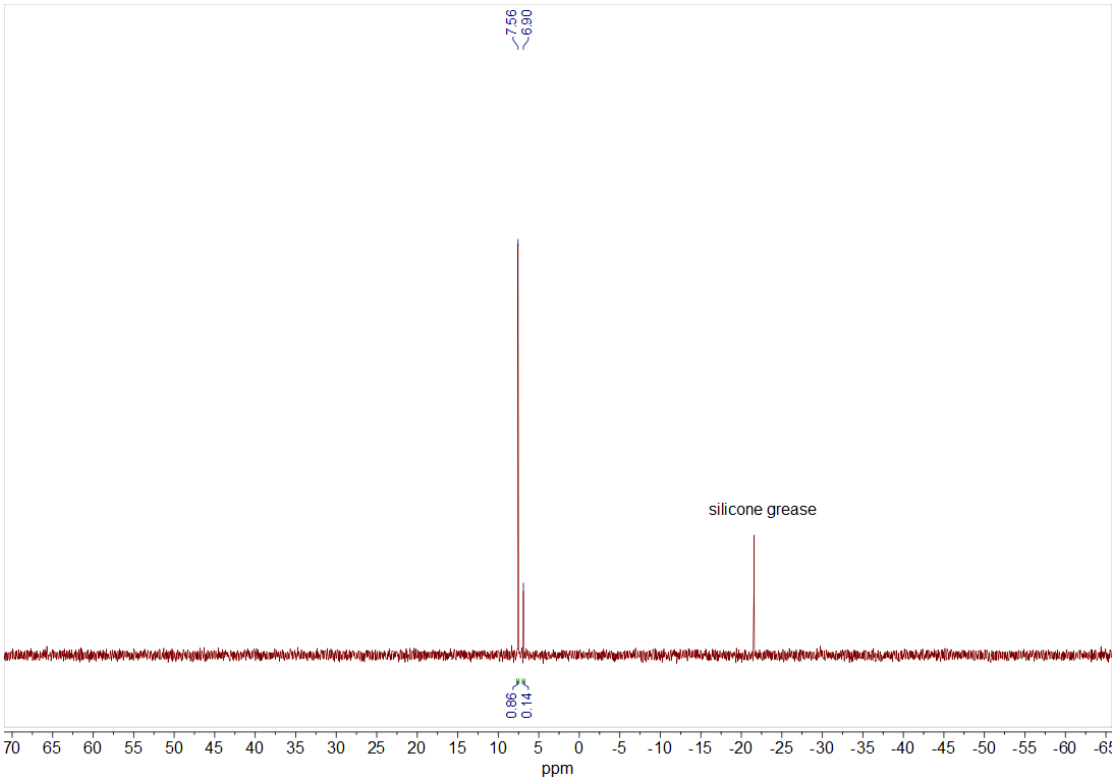
HMBC (^{1}H, ^{13}C) (THF-d_8, -40 °C) for ^{13}C NMR of CH_{NiPr} (δ 54.4):



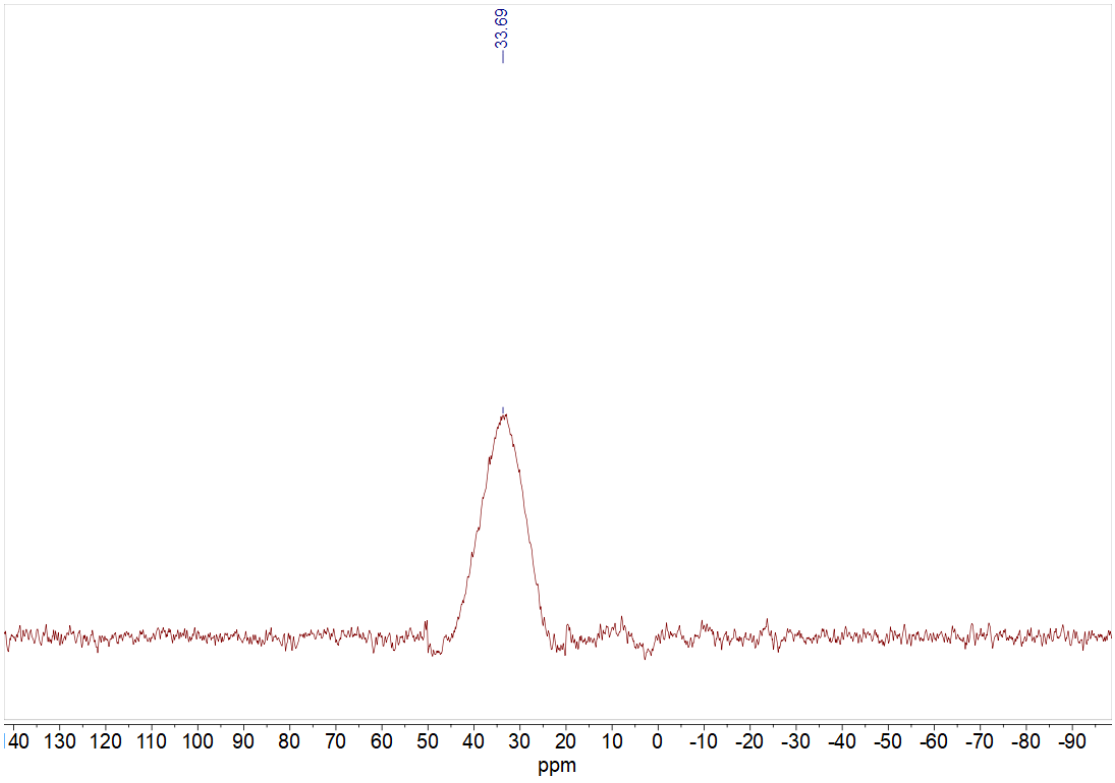
^{31}P{^{1}H} NMR (162 MHz, THF-d_8, -40 °C):

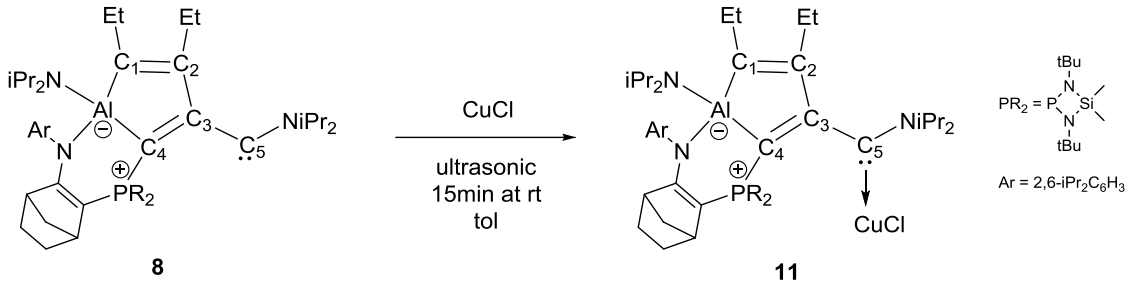


$^{29}Si\{^{1}H\}$ NMR (80 MHz, THF-d_8, -40 °C):



$^{11}B\{^{1}H\}$ NMR (128 MHz, THF-d_8, -40 °C):





Synthesis of 11: To **8** (200 mg, 0.214 mmol) and CuCl (22 mg, 0.214 mmol), toluene (2 ml) was added at room temperature and the solution was ultrasonicated for 15 minutes at room temperature. Then, all volatiles were removed under vacuum. The crude products were washed by acetonitrile (5ml X 3). The resulting solid was dried under vacuum to obtain **11** as orange powders (175 mg, yield = 80 %). Crystals suitable for X-ray diffraction analysis were obtained from the slow evaporation of a saturated benzene solution at –25 °C. Ratio major/minor isomers 4:1. Mp: 167 -170 °C (decomp.).

Major diastereomer (80 %)

^{1}H NMR (400 MHz, C_6D_6, 25 °C): δ 0.33 (s, 3H, $SiCH_3$), 0.77 - 0.86 (m, 6H, CH_{3Et} and CH_{3NiPr}), 0.80 (s, 3H, $SiCH_3$), 0.82 (m, 3H, $CH_{3AlNiPr}$), 0.93 (d, J_{HH} = 6.5 Hz, 3H, CH_{3NiPr}), 1.14 (s, 9H, CH_{3tBu}), 1.16 (m, 3H, CH_{3iPr}), 1.17 (m, 1H, CH_2), 1.28 (m, 3H, CH_{3iPr}), 1.29 (m, 3H, CH_{3Et}), 1.32 (m, 1H, CH_2), 1.33 (d, J_{HH} = 6.7 Hz, 3H, $CH_{3AlNiPr}$), 1.40 (d, J_{HH} = 6.9 Hz, 6H, $CH_{3AlNiPr}$), 1.45 (m, 1H, CH_2), 1.46 (d, J_{HH} = 6.7 Hz, 3H, CH_{3iPr}), 1.55 (m, 1H, CH_2), 1.56 (d, J_{HH} = 6.6 Hz, 3H, CH_{3iPr}), 1.69 (d, J_{HH} = 6.9 Hz, 3H, CH_{3NiPr}), 1.80 (s, 9H, CH_{3tBu}), 1.81 (s, 3H, CH_{3NiPr}), 1.93 (d, J_{HH} = 8.4 Hz, 1H, CH_2), 2.03 (m, 1H, CH_2), 2.12– 2.25 (m, 2H, CH_{2Et}), 2.33 (m, 2H, CH_{2Et}), 2.87 (br, 1H, $CH_{bridgehead}$), 3.09 (br, 1H, $CH_{bridgehead}$), 3.53 (m, 2H, CH_{NiPr} and CH_{iPr}), 3.80 (sept, J_{HH} = 6.8 Hz, 2H, CH_{AlNiPr}), 4.58 (m, J_{HH} = 6.5 Hz, 2H, CH_{NiPr} and CH_{iPr}), 7.17-7.32 (m, 3H, CH_{Ar}).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 25 °C): δ 4.9 (s, $SiCH_3$), 7.8 (d, J_{CP} = 1.8 Hz, $SiCH_3$), 15.0 (s, CH_{3Et}), 16.6 (s, CH_{3Et}), 19.3 (s, $CH_{3AlNiPr}$), 21.4 (s, $CH_{3AlNiPr}$), 23.9 (s, CH_{3iPr}), 24.4 (s, CH_{3NiPr} x 2), 24.6 (s, CH_2), 25.3 (s, CH_{2Et}), 25.6 (s, CH_{2Et}), 25.6 (s, CH_{3iPr}), 25.7 (s, CH_{3iPr}), 26.7 (s, CH_{3iPr}), 28.2 (s, CH_2), 28.3 (s, $CH_{3AlNiPr}$ x 2), 28.7 (br, CH_{3NiPr} x 2), 33.1 (d, J_{CP} = 5.0 Hz, CH_{3tBu}), 34.5 (d, J_{CP} = 4.8 Hz, CH_{3tBu}), 45.4 (d, J_{CP} = 14.3 Hz, $CH_{bridgehead}$), 48.0 (d, J_{CP} = 9.6 Hz, CH_2), 48.9 (d, J_{CP} = 11.9 Hz, $CH_{bridgehead}$), 50.6 (br, CH_{AlNiPr} X 2), 51.7 (s, C_{tBu}), 53.0 (s, CH_{NiPr}), 53.6 (s, C_{tBu}), 58.6 (s, CH_{NiPr}), 95.5 (d, J_{CP} = 144.9 Hz, CP), 124.2 (s, CH_{Ar}), 125.1 (s, CH_{Ar}), 126.5 (s, CH_{Ar}), 137.8 (br, Al-C_4-P), 144.3 (s, N-C_{Ar}), 145.8 (s, iPr-C_{Ar}), 146.7 (s, iPr-C_{Ar}), 152.2 (d, J_{CP} = 30.5 Hz, Et-C_2), 175.3 (br, Al-C_1-Et), 176.7 (d, J_{CP} = 13.0 Hz, C_3), 186.4 (d, J_{CP} = 7.9 Hz, NC), 241.5 (d, J_{CP} = 17.3 Hz, Cu-C_5).

^{31}P{^{1}H} NMR (162 MHz, C_6D_6, 25 °C): δ 20.6 (s, CP).

^{29}Si{^{1}H} NMR (80 MHz, C_6D_6, 25 °C): δ 4.9 (s, $SiCH_3$).

Minor diastereomer (20 %)

^{1}H NMR (400 MHz, C_6D_6, 25 °C): δ 0.34 (s, 3H, $SiCH_3$), 0.37 (s, 3H, $SiCH_3$), 0.57 (t, J_{HH} = 7.0 Hz, 3H, CH_{3Et}), 0.78 (m, 6H, CH_{3NiPr}), 0.95 (m, 1H, CH_2), 1.21 (m, 3H, $CH_{3AlNiPr}$), 1.23 (s, 9H, CH_{3tBu}), 1.31 (m, 3H, CH_{3iPr}), 1.35 (m, 3H, CH_{3iPr}), 1.38 (m, 3H, $CH_{3AlNiPr}$), 1.39 (d, J = 7.3 Hz, 6H, $CH_{3AlNiPr}$), 1.48 (m, 3H, CH_{3Et}), 1.49 (m, 1H, CH_2), 1.56 (m, 1H, CH_2), 1.60 (d, J = 6.6 Hz, 6H, CH_{3iPr}), 1.66 (m, 1H, CH_2), 1.71 (m, 1H, CH_2), 1.73 (m, 3H, CH_{3NiPr}), 1.75 (s, 9H, CH_{3tBu}), 1.78 (m,

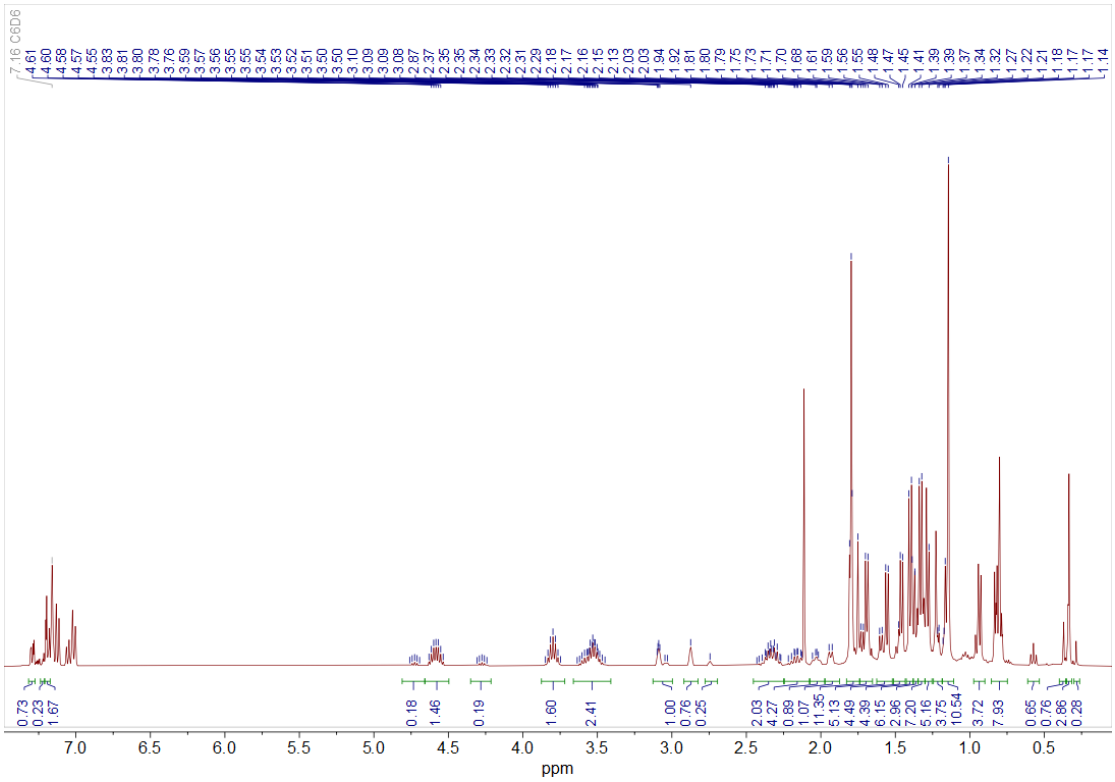
3H, $CH_{3N\textit{i}Pr}$), 1.93 (d, *J* = 8.4 Hz, 1H, CH_2), 2.25 – 2.12 (m, 2H, CH_{2Et}), 2.36 (m, 2H, CH_{2Et}), 2.74 (br, 1H, $CH_{bridgehead}$), 3.04 (d, *J* = 7.1 Hz, 1H, $CH_{bridgehead}$), 3.57 (sept, *J* = 6.8 Hz, 2H, $CH_{AlN\textit{i}Pr}$), 3.58 (m, 2H, $CH_{N\textit{i}Pr}$ and $CH_{\textit{i}Pr}$), 4.27 (sept, *J* = 6.7 Hz, 1H, $CH_{\textit{i}Pr}$), 4.73 (sept, *J* = 6.7 Hz, 1H, $CH_{N\textit{i}Pr}$), 7.17 -7.32 (m, 3H, CH_{Ar}).

$^{13}C\{^1H\}$ NMR (101 MHz, C_6D_6, 25 °C): δ 5.5 (s, $SiCH_3$), 7.3 (d, J_{CP} = 2.7 Hz, $SiCH_3$), 15.0 (s, CH_{3Et}), 15.9 (s, CH_{3Et}), 18.4 (s, $CH_{3AlN\textit{i}Pr}$), 22.5 (s, $CH_{3AlN\textit{i}Pr}$), 23.7 (s, CH_2), 24.3 (s, CH_{3NiPr} X 2), 25.1 (s, $CH_{3\textit{i}Pr}$), 25.8 (s, $CH_{3\textit{i}Pr}$), 26.0 (s, $CH_{3\textit{i}Pr}$), 26.4 (d, J_{CP} = 1.8 Hz, CH_{2Et}), 26.6 (s, $CH_{3\textit{i}Pr}$), 28.0 (s, $CH_{3N\textit{i}Pr}$ X 2), 28.8 (s, $CH_{3AlN\textit{i}Pr}$ X 2), 29.1 (s, CH_2), 33.8 (d, J_{CP} = 4.9 Hz, CH_{3tBu}), 34.7 (d, J_{CP} = 4.6 Hz, CH_{3tBu}), 44.4 (d, J_{CP} = 15.6 Hz, $CH_{bridgehead}$), 44.8 (d, J_{CP} = 4.6 Hz, CH_2), 47.7 (d, J_{CP} = 11.1 Hz, $CH_{bridgehead}$), 47.9 (br, CH_{AlNiPr} X2), 51.7 (s, C_{tBu}), 52.9 (s, CH_{NiPr}), 53.3 (s, C_{tBu}), 57.0 (s, CH_{NiPr}), 93.7 (d, J_{CP} = 143.3 Hz, CP), 124.7 (s, CH_{Ar}), 125.2 (s, CH_{Ar}), 126.0 (s, CH_{Ar}), 137.8 (br, Al-C_4-P), 144.6 (s, N-C_{Ar}), 145.2 (s, iPr-C_{Ar}), 146.9 (s, iPr-C_{Ar}), 148.3 (d, J_{CP} = 32.0 Hz, Et-C_2), 172.4 (d, J_{CP} = 11.6 Hz, C_3), 175.3 (br, Al-C_1-Et), 185.1 (d, J_{CP} = 7.6 Hz, NC), 244.4 (d, J_{CP} = 14.4 Hz, Cu-C_5).

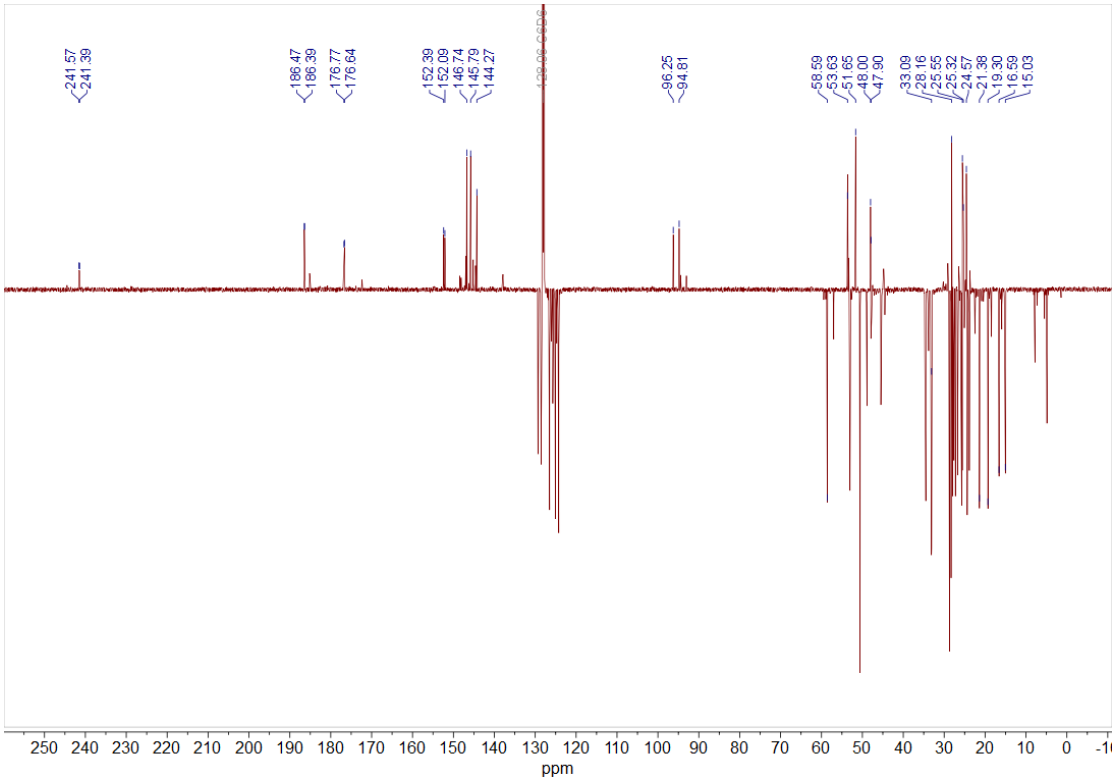
$^{31}P\{^1H\}$ NMR (162 MHz, C_6D_6, 25 °C): δ 27.7 (s, CP).

$^{29}Si\{^1H\}$ NMR (80 MHz, C_6D_6, 25 °C): δ 5.7 (s, $SiCH_3$).

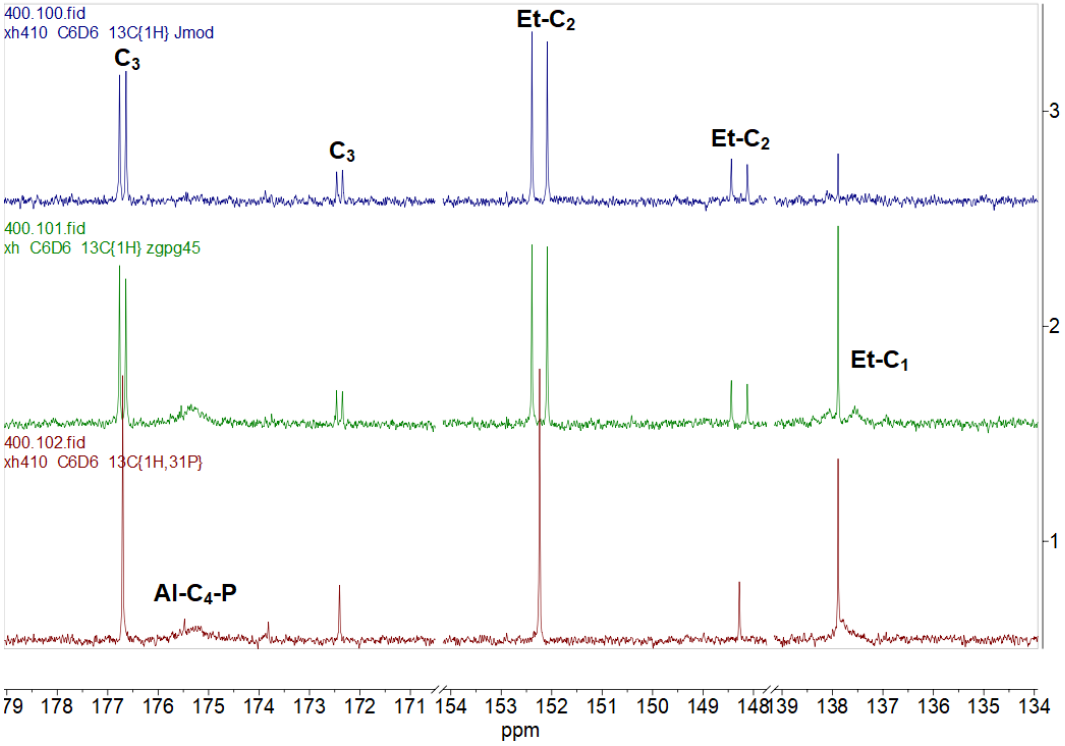
^{1}H NMR (400 MHz, C_6D_6, 25 ^{o}C):



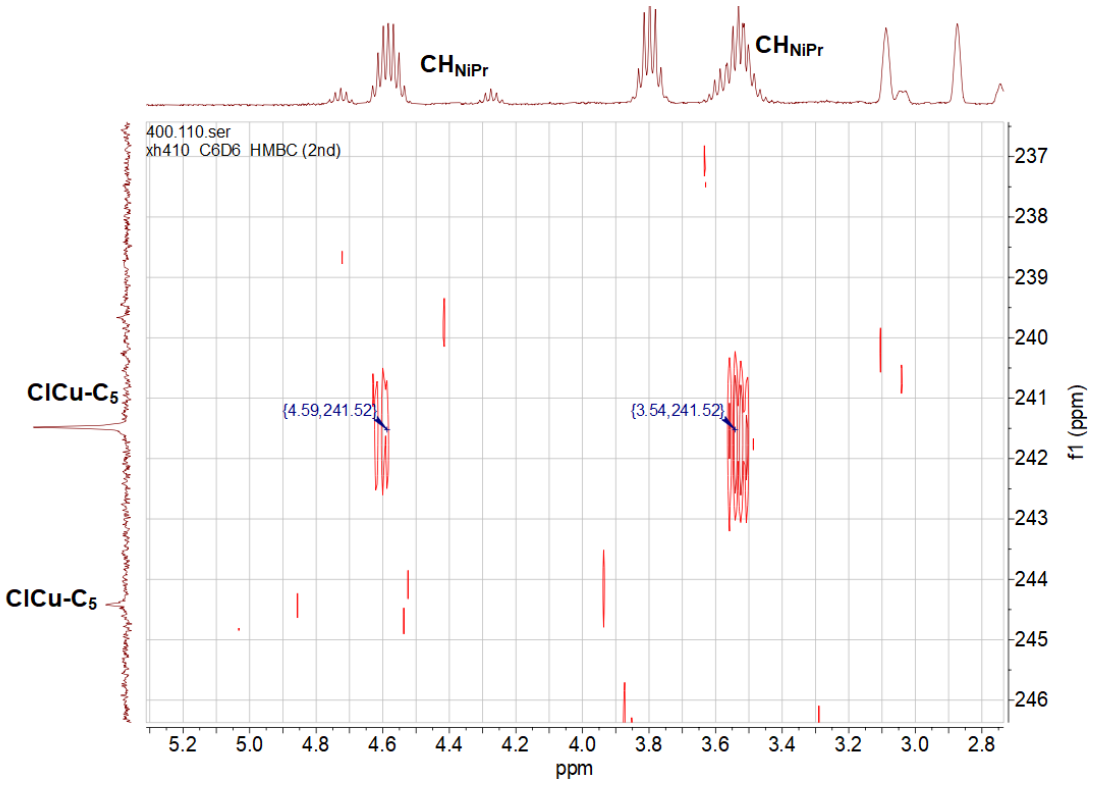
^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 25 ^{o}C):



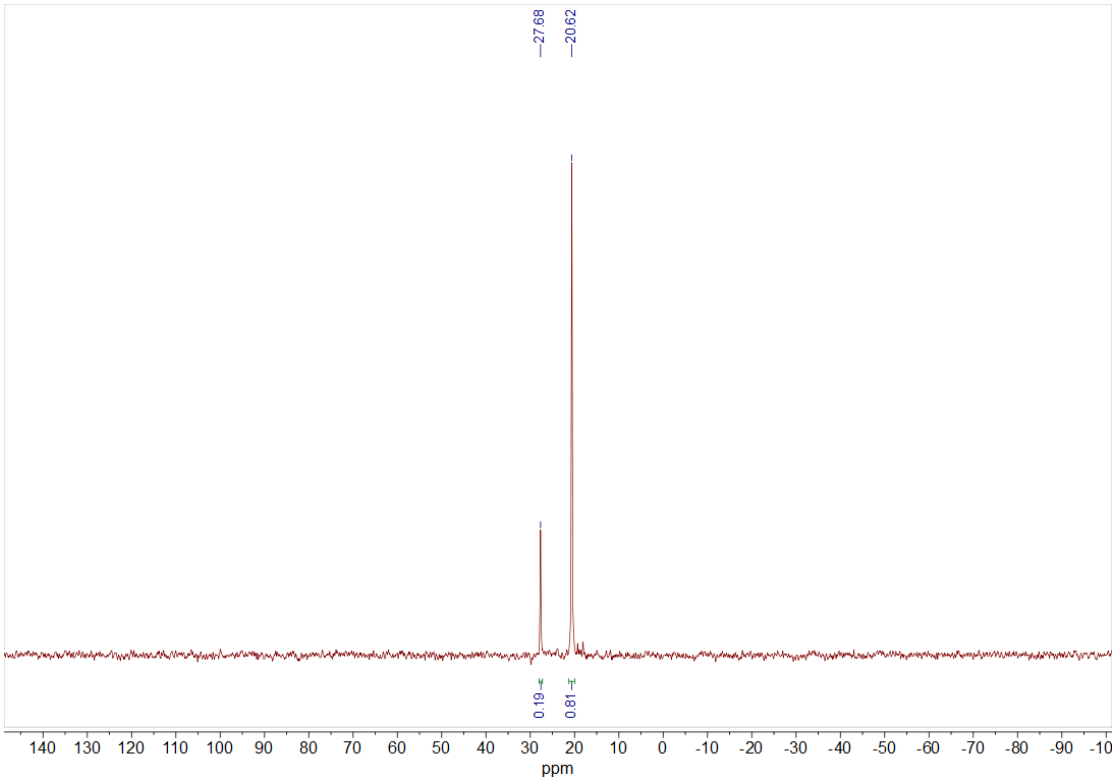
$^{13}C\{^{1}H\}$-NMR (upside) and $^{13}C\{^{1}H,^{31}P\}$-NMR (downside) (101 MHz, C_6D_6, 25 °C):



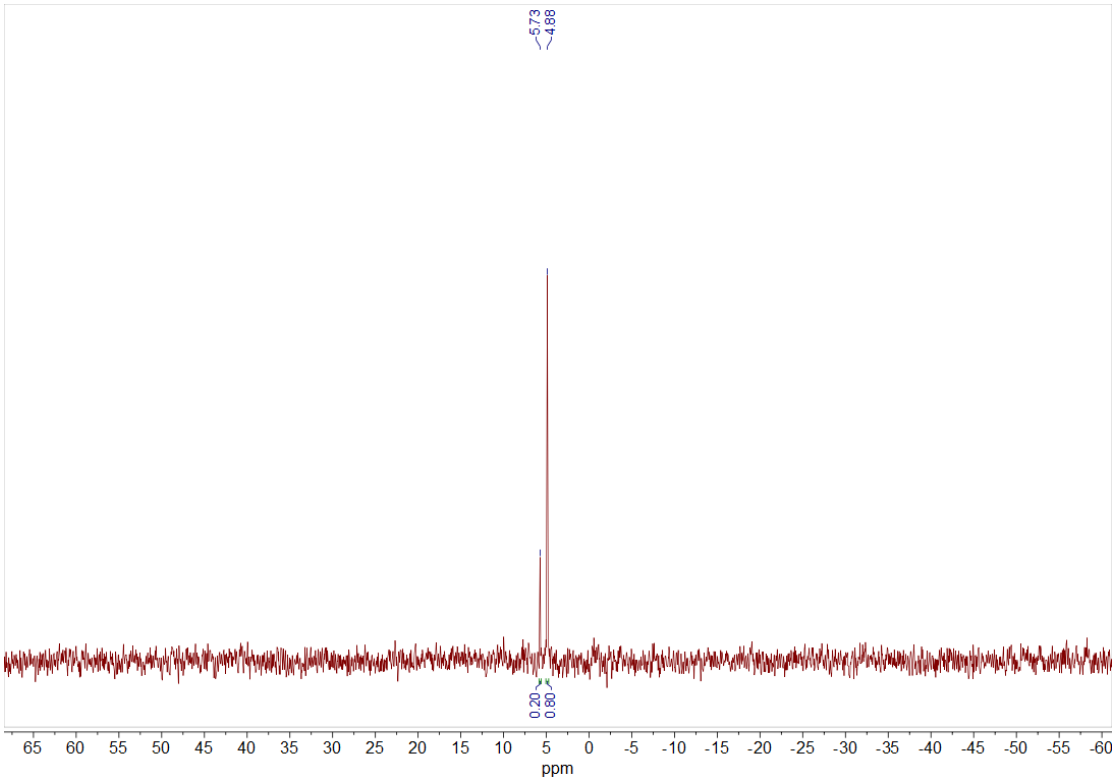
HMBC (^{1}H, ^{13}C) (C_6D_6, 25 °C) for ^{13}C NMR of CuC_5 (δ 241.5; δ 244.4):



$^{31}P\{^{1}H\}$ NMR (162 MHz, C_6D_6, 25 ^{o}C):



$^{29}Si\{^{1}H\}$ NMR (80 MHz, C_6D_6, 25 ^{o}C):



3-Crystallographic data collection and structure determination:

The data collection was performed at low temperature (193 K) using MoKα radiation (λ = 0.71073 Å) on a Bruker-AXS APEX II CCD Quazar diffractometer equipped with a 30 W air-cooled microfocus source (**5**, **6**, **8** and **9**), on a Bruker-AXS D8-Venture equipped with a Bruker PHOTON III-C14 detector (**1**, **3**) or on a Bruker-AXS D8-Quest with a microfocus sealed tube using a multilayer mirror as monochromator and a Bruker PHOTON III-C14 CPAD detector (**11**). Phi- and omega- scans were used. The data were integrated with SAINT (S2) and an empirical absorption correction with SADABS was applied (S3). The structures were solved using an intrinsic phasing method (SHELXT) (S4) and refined using a least-squares method on *F*2 (S5). All non-H atoms were refined with anisotropic displacement parameters. Hydrogen atoms were refined isotropically at calculated positions using a riding model with their isotropic displacement parameters constrained to be equal to 1.5 times the equivalent isotropic displacement parameters of their pivot atoms for terminal sp^3 carbon and 1.2 times for all other carbon atoms.

Structures of compounds **1**, **6**, **9** and **11** were found to be disordered. Several restraints (SAME, SIMU, DELU/RIGU, SADI) and equal xyz and U_{ij} constraints (EXYZ and EADP) (**11**) were applied to refine some moieties of the molecules and to avoid the collapse of the structures during the least-squares refinement by the large anisotropic displacement parameters. Some residual electron density were difficult to modelize in structure of compound **8** and therefore, the SQUEEZE function of PLATON (S6) was used to eliminate the contribution of the electron density in the solvent region from the intensity data, and the solvent-free model was employed for the final refinement.

CCDC-2441055 (**1**), CCDC-2441056 (**3**), CCDC-2441057 (**5**), CCDC-2441058 (**6**), CCDC-2441059 (**8**), CCDC-2441060 (**9**) and CCDC-2441061 (**11**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via https://www.ccdc.cam.ac.uk/structures/.

	1	**3**	**5**	**6**	**8**	**9**	**11**
CCDC number	2441055	2441056	2441057	2441058	2441059	2441060	2441061
Empirical formula	$C_{75}H_{130}Al_2N_6P_2Si_2$	$C_{46}H_{79}AlN_5PSi$	$C_{46}H_{79}AlN_5PSi$	$C_{46}H_{79}AlN_5PSi$	$C_{50}H_{87}AlN_5PSi$	$C_{62}H_{101}AlN_5OPSi$	$C_{62}H_{99}AlClCuN_5PSi$
Formula weight	1287.92	788.18	788.18	788.18	844.28	1018.51	1099.49
Temperature [K]	193(2)	193(2)	193(2)	193(2)	193(2)	193(2)	193(2)
Crystal system	triclinic	monoclinic	monoclinic	monoclinic	monoclinic	triclinic	monoclinic
Space group	$P\overline{1}$	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/c$	$P\overline{1}$	$P2_1/c$
a [Å]	10.4696(7)	12.1189(12)	12.6590(10)	13.8960(14)	15.9863(9)	12.0584(9)	24.8337(12)
b [Å]	10.7334(7)	21.9059(16)	17.5105(12)	17.3957(16)	17.6296(10)	13.9968(9)	10.5705(5)
c [Å]	19.3518(13)	18.1582(17)	20.6407(15)	19.5978(17)	18.6567(11)	18.0629(13)	25.3214(12)
α [°]	91.039(2)	90	90	90	90	90.561(2)	90
β [°]	104.121(2)	100.850(4)	90.190(3)	104.351(3)	95.958(2)	92.765(2)	109.228(2)
γ [°]	105.729(2)	90	90	90	90	98.516(2)	90
Volume [Å^3]	2021.7(2)	4734.4(7)	4575.3(6)	4589.6(7)	5229.7(5)	3011.1(4)	6276.2(5)
Z	1	4	4	4	4	2	4
ρ_{calc} [gcm^{-3}]	1.058	1.106	1.144	1.141	1.072	1.123	1.164
μ [mm^{-1}]	0.146	0.137	0.142	0.142	0.128	0.123	0.489
Reflections collected	73223	179404	116536	75496	165290	91728	167766
Independent reflections	10097 R_{int} = 0.0714 R_{sigma} = 0.0415	12287 R_{int} = 0.0607 R_{sigma} = 0.0253	11383 R_{int} = 0.0805 R_{sigma} = 0.0500	7286 R_{int} = 0.2477 R_{sigma} = 0.1574	12500 R_{int} = 0.0909 R_{sigma} = 0.0495	12350 R_{int} = 0.0888 R_{sigma} = 0.0683	15556 R_{int} = 0.1221 R_{sigma} = 0.0529
Data/Restraints/Parameters	10097 / 347 / 500	12287 / 0 / 507	11383 / 0 / 507	7286 / 144 / 541	12500 / 0 / 545	12350 / 464 / 755	15556 / 1218 / 859
Goodness-of-fit on F^2	1.021	1.012	1.026	1.035	1.012	1.047	1.046
Final *R* indexes	R_1 = 0.0572	R_1 = 0.0361	R_1 = 0.0458	R_1 = 0.1028	R_1 = 0.0533	R_1 = 0.0661	R_1 = 0.0606

[$I \geq 2\sigma(I)$]	wR_2 = 0.1532	wR_2 = 0.0916	wR_2 = 0.1026	wR_2 = 0.2089	wR_2 = 0.1247	wR_2 = 0.1736	wR_2 = 0.1494
Final *R* indexes [all data]	R_1 = 0.0877 wR_2 = 0.1758	R_1 = 0.0505 wR_2 = 0.1013	R_1 = 0.0799 wR_2 = 0.1197	R_1 = 0.2300 wR_2 = 0.2851	R_1 = 0.0922 wR_2 = 0.1462	R_1 = 0.1175 wR_2 = 0.2024	R_1 = 0.0920 wR_2 = 0.1714
Largest peak/hole [eÅ^{-3}]	0.90/−0.32	0.35/−0.30	0.44/−0.28	0.51/−0.58	0.85/−0.39	0.63/−0.42	0.76/−0.53

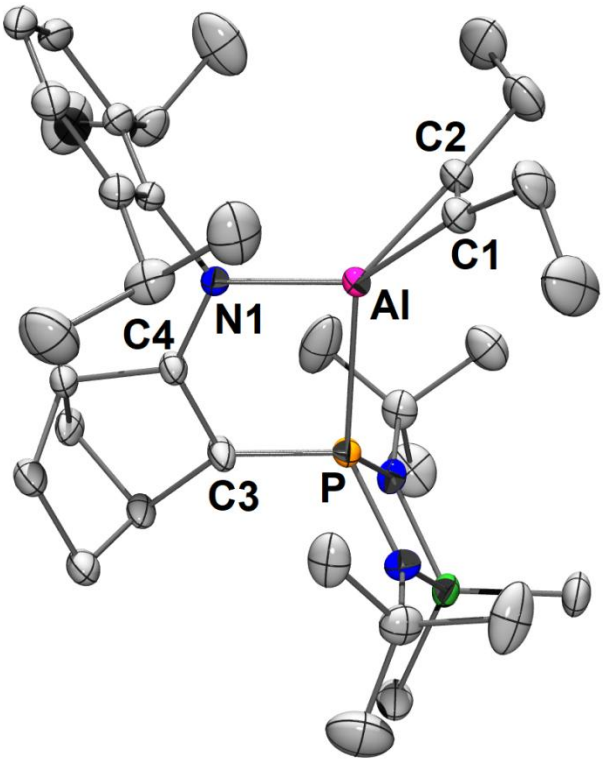


Figure S1. Molecular structure of **1**. Thermal ellipsoids represent 30 % probability. H and disordered atoms and solvent molecules (pentane) are omitted for clarity. Selected bond lengths [Å] and angles [°]: Al-C1 1.899(2), C1-C2 1.358(3), C2-Al 1.876(2), N1-Al 1.888(2), Al-P 2.420(1), P-C3 1.722(2), C3-C4 1.383(3), C4-N1 1.348(2), C1-Al-C2 42.16(11), Al-C1-C2 68.02(13), C1-C2-Al 69.82(13), N1-Al-P 88.06(5), Al-P-C3 92.69(7), P-C3-C4 117.40(15), C3-C4-N1 126.90(18).

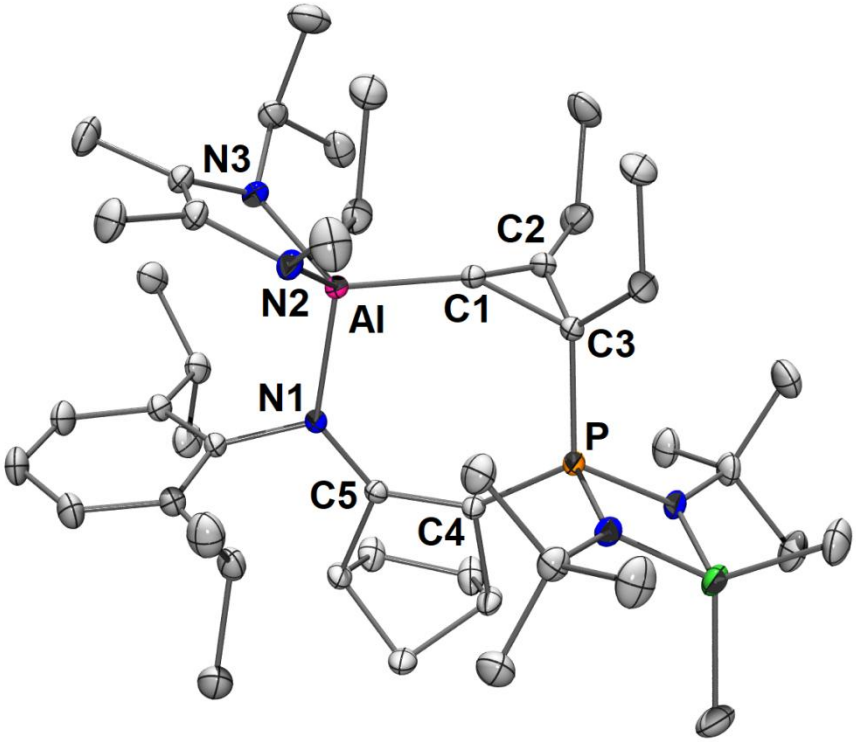


Figure S2. Molecular structure of **3**. Thermal ellipsoids represent 30 % probability. H atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Al-N2 1.841(1), Al-N3 1.842(1), N1-Al 1.936(1), Al-C1 1.959(1), C1-C2 1.298(2), C2-C3 1.501(2), C3-C1 1.583(2), C3-P 1.789(1), P-C4 1.754(1), C4-C5 1.414(2), C5-N1 1.360(1), N2-Al-N3 93.10(5), N1-Al-C1 99.10(4), Al-C1-C2 153.39(10), Al-C1-C3 140.11(9), C3-C1-C2 61.89(8), C1-C2-C3 68.44(9), C2-C3-C1 49.67(7), C1-C3-P 114.98(8), C2-C3-P 118.76(9), C3-P-C4 113.47(5), P-C4-C5 138.62(9), C4-C5-N1 135.32(10), C5-N1-Al 131.69(7). Σ°_{N2} = 340.90°. Σ°_{N3} = 352.62°. Σ°_{C1} = 355.39°.

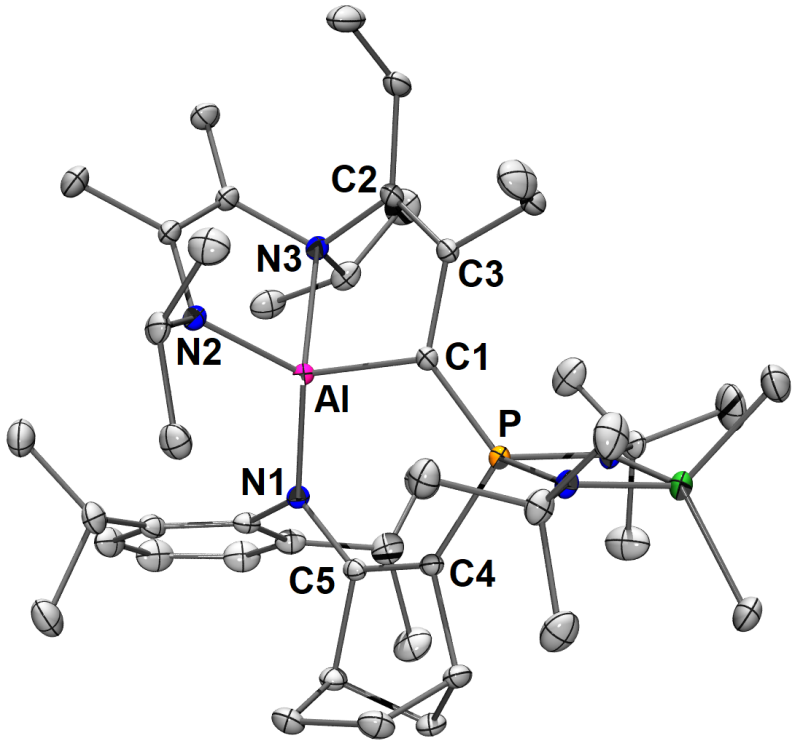


Figure S3. Molecular structure of **5**. Thermal ellipsoids represent 30 % probability. H atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Al-N1 1.886(2), Al-N2 1.850(2), Al-N3 2.026(2), Al-C1 1.895(2), C1-C3 1.463(2), C3-C2 1.361(3), C2-N3 1.507(2), C1-P 1.670(2), P-C4 1.774(2), C4-C5 1.378(2), C5-N1 1.388(2), N3-Al-C1 90.96(7), Al-C1-C3 104.68(12), C2-N3-Al 100.47(10), C1-C3-C2 120.35(16), C3-C2-N3 117.42(15), N3-Al-N2 86.66(6), Al-C1-P 122.76(10), P-C1-C3 131.03(13), C1-P-C4 105.15(8), P-C4-C5 130.19(13), C4-C5-N1 131.27(15), C5-N1-Al 113.88(11), N1-Al-C1 108.23(7), N1-Al-N2 120.12(7).

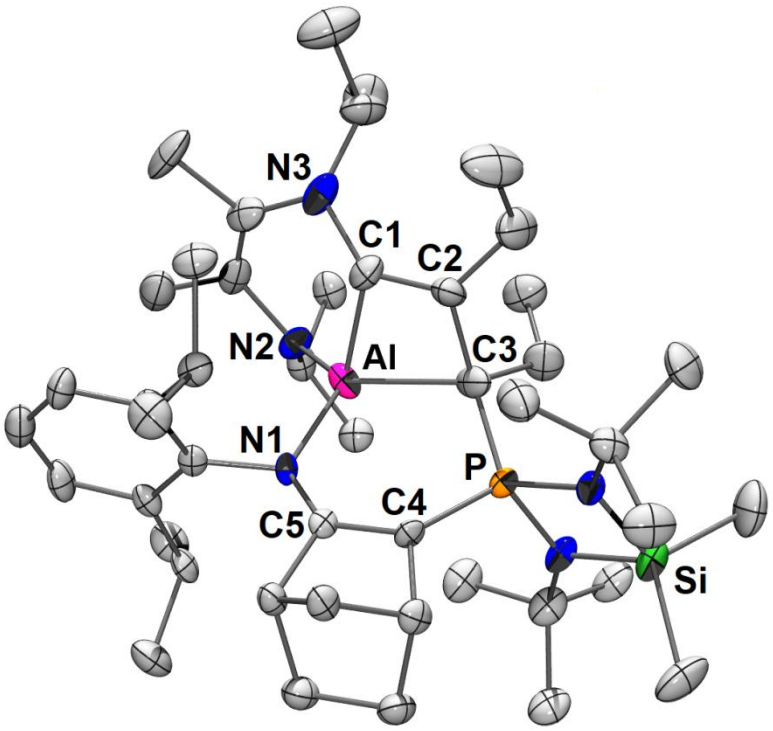


Figure S4. Molecular structure of **6**. Thermal ellipsoids represent 30 % probability. H and disordered atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: C1-N3 1.398(9), C1-Al 1.849(8), Al-N2 1.821(7), Al-C3 2.145(8), C3-C2 1.534(10), C2-C1 1.400(10), C3-P 1.824(8), P-C4 1.739(7), C4-C5 1.368(9), C5-N1 1.349(8), N1-Al 1.865(6), Al-C3-C2 82.6(4), C3-C2-C1 106.5(7), C2-C1-N3 135.2(8), N3-C1-Al 124.2(6), C2-C1-Al 98.0(5), C1-Al-C3 71.7(3), Al-C3-P 113.4(4), C3-P-C4 109.2(3), P-C4-C5 132.4(5), C5-N1-Al 123.6(4).

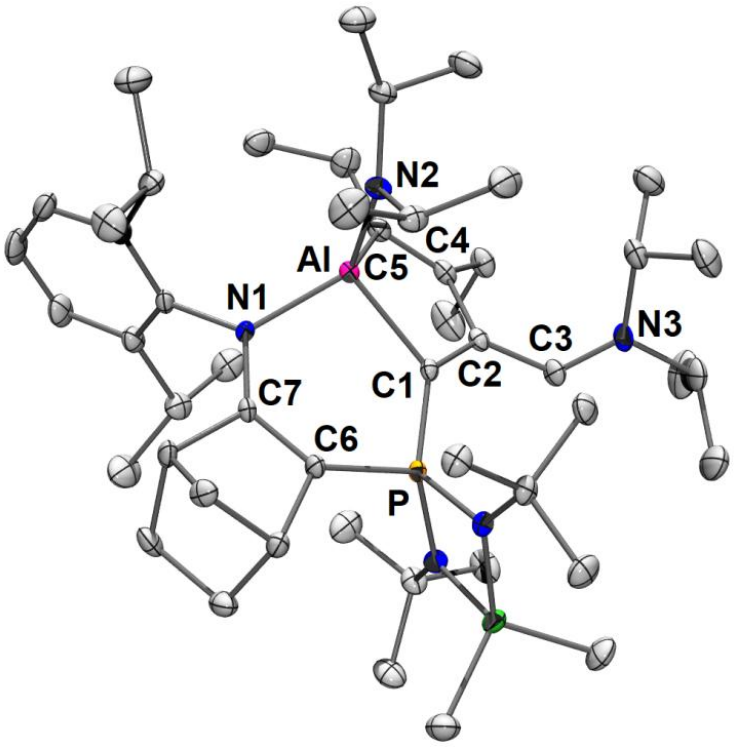


Figure S5. Molecular structure of **8**. Thermal ellipsoids represent 30 % probability. H atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: Al-C1 1.992(2), C1-C2 1.401(3), C1-P 1.708(2), C2-C3 1.415(3), C3-N3 1.285(3), C2-C4 1.518(3), C4-C5 1.355(3), C5-Al 1.990(2), N1-Al 1.917(2), Al-N2 1.845(2), C2-C3-N3 125.7(2), Al-C1-P 122.4(1), P-C1-C2 133.6(2), Al-C1-C2 103.2(2), C1-C2-C3 125.6(2), C3-C2-C4 116.6(2), C1-C2-C4 117.6(2), C2-C4-C5 117.9(2), C4-C5-Al 106.3(2), C5-Al-C1 90.2(1).

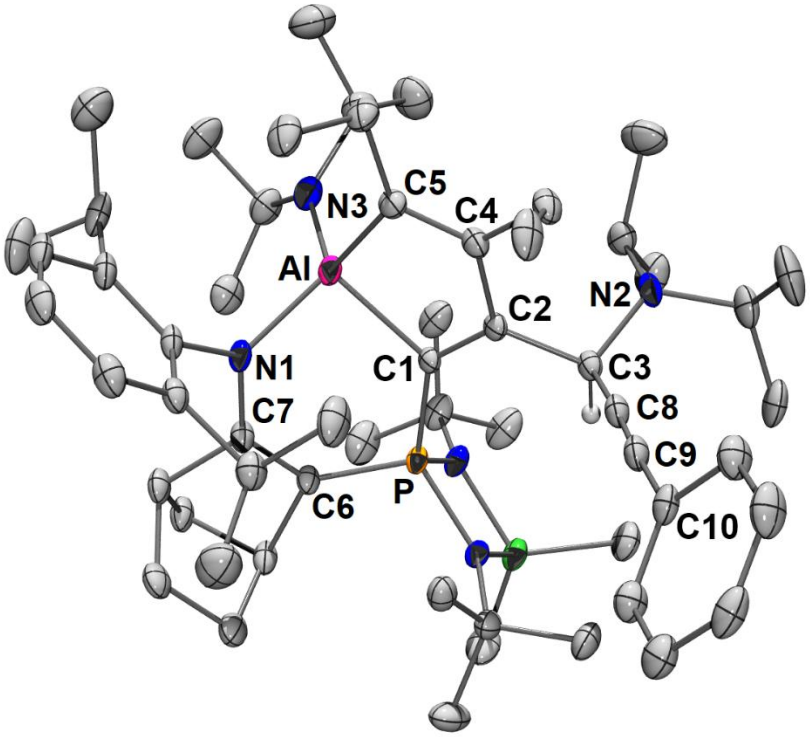


Figure S6. Molecular structure of **9**. Thermal ellipsoids represent 30 % probability. H and disordered atoms and solvent molecules (THF) are omitted for clarity. Selected bond lengths [Å] and angles [°]: Al-C1 2.026(3), C1-C2 1.375(4), C2-C3 1.546(4), C2-C4 1.520(4), C4-C5 1.355(4), C5-Al 1.982(3), C1-P1 1.744(3), P-C6 1.754(3), C6-C7 1.399(4), C7-N1 1.354(4), N1-Al 1.907(3), C3-N2 1.485(4), C3-C8 1.471(4), C8-C9 1.185(4), Al1-N3 1.856(3), Al-C1-C2 106.6(2), P-C1-C2 132.6(2), C1-C2-C4 118.0(2), C1-C2-C3 123.6(2), C3-C2-C4 118.4(2), C2-C4-C5 117.2(3), C4-C5-Al 109.2(2), C5-Al-C1 88.1(1), C5-Al-N1 116.9(1), N1-Al-C1 98.2(1), Al-C1-P 120.3(2), C1-P-C6 102.2(1), P-C6-C7 131.4(2), C6-C7-N1 131.5(3), C7-N1-Al 116.5(2), C2-C3-N2 109.4(2), C3-C8-C9 176.7(3), C8-C9-C10 177.1(3).

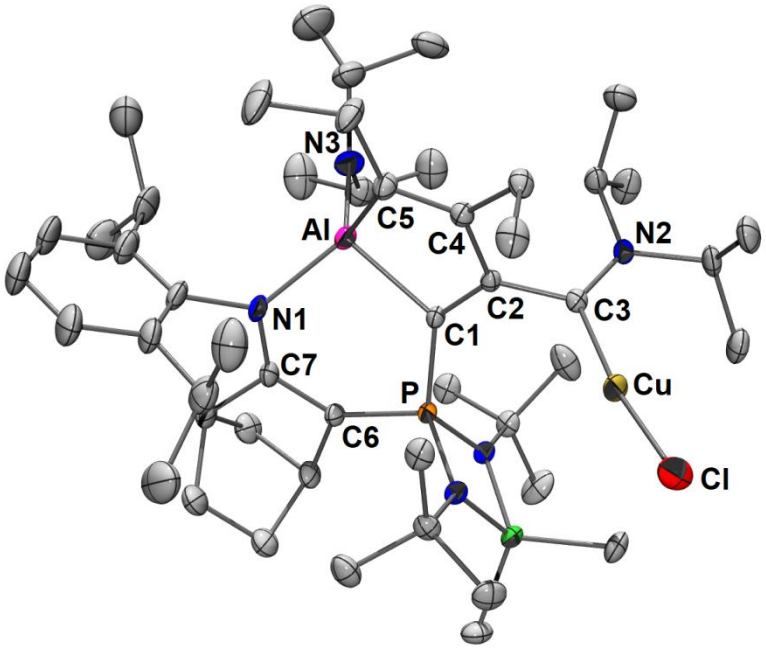


Figure S7. Molecular structure of **11**. Thermal ellipsoids represent 30 % probability. H and disordered atoms and solvent molecules (C_6D_6) are omitted for clarity. Selected bond lengths [Å] and angles [°]: Al-C1 2.026(3), C1-C2 1.379(4), C2-C3 1.483(4), C3-N2 1.308(3), C3-Cu 1.896(3), Cu-Cl 2.121(1), C2-C4 1.511(4), C4-C5 1.354(4), C5-Al 1.994(3), C1-P 1.737(3), P-C6 1.748(3), C6-C7 1.398(4), C7-N1 1.355(4), N1-Al 1.908(3), Al-N3 1.838(3), Al-C1-C2 104.3(2), P-C1-C2 133.2(2), C1-C2-C4 117.6(2), C1-C2-C3 126.6(2), C3-C2-C4 115.8(2), C2-C3-N2 118.5(2), N2-C3-Cu 122.9(2), Cu-C3-C2 117.8(2), C3-Cu-Cl 169.4(1), C2-C4-C5 118.1(2), C4-C5-Al 107.0(2), C5-Al-C1 88.1(1), C5-Al-N1 123.0(2), N1-Al-C1 103.2(1), Al-C1-P 121.4(2), C1-P-C6 103.9(1), P-C6-C7 131.2(2), C6-C7-N1 131.3(3), C7-N1-Al 115.2(2).

4-Computational details

Geometries of all systems have been optimized with the Gaussian-16 program (S17) using the M06-2X density functional (S28) and the 6-31G(d) basis set. Harmonic vibrational frequencies were calculated in order to verify that these structures correspond to energy minima (all frequencies are real) or transition structures (one and only one imaginary frequency). Energies of all structures were recalculated through single point calculations with the Def2-TZVP basis set.(S3[9]) The reported Gibbs energies at 298 K and 1 atm have been computed from energies at the M06-2X/Def2-TZVP level of calculation and zero-point vibrational, thermal and entropy contributions computed at the M06-2X/6-31G(d) level. For the triplet states a spin unrestricted formalism has been adopted.

Total energies and Gibbs energies (in a.u.)

	M06-2X/6-31G(d)		M06-2X/Def2TZVP//M06-2X/6-31G(d)
	E	G	E
1	-2406.056428	-2405.248948	-2406.741968
2	-540.4263824	-540.166219	-540.63551
INT1	-2946.526377	-2945.422493	-2947.409467
TS(INT1-->INT2)	-2946.501098	-2945.397027	-2947.385325
INT2	-2946.52816	-2945.425325	-2947.410926
TS(INT2-->INT3)	-2946.499691	-2945.39883	-2947.383255
INT3	-2946.536196	-2945.434709	-2947.418047
TS(INT3-->6)	-2946.518239	-2945.416172	-2947.400646
6	-2946.548176	-2945.440755	-2947.435541
TS(INT3-->INT4)	-2946.499317	-2945.396124	-2947.383464
INT4	-2946.520296	-2945.41626	-2947.405954
TS(INT4-->INT5)	-2946.505171	-2945.40384	-2947.389688
INT5	-2946.552274	-2945.445966	-2947.444539
TS(INT5-->4)	-2946.522203	-2945.421133	-2947.409509
4	-2946.530017	-2945.430735	-2947.417412
TS(4-->3)	-2946.512805	-2945.412169	-2947.400013
3	-2946.558892	-2945.454047	-2947.448801
TS(INT5-->5)	-2946.502482	-2945.400883	-2947.394937
5	-2946.609978	-2945.498741	-2947.499089
7	-697.51221	-697.147555	-697.7810727
7 -triplet	-697.4021048	-697.041702	-697.6685847
INT6	-3103.623735	-3102.413204	-3104.566784
TS(INT6-->INT7)	-3103.596736	-3102.39148	-3104.539198
INT7	-3103.632933	-3102.42119	-3104.575057
TS(INT7-->INT8)	-3103.617293	-3102.405189	-3104.561083
INT8	-3103.623462	-3102.415029	-3104.567817
TS(INT8-->INT9)	-3103.595611	-3102.386822	-3104.537828
INT9	-3103.661749	-3102.449067	-3104.602966

TS(INT9-->INT10)	-3103.609964	-3102.402585	-3104.549055
INT10	-3103.664966	-3102.456017	-3104.60687
TS(INT10-->INT11)	-3103.65376	-3102.439894	-3104.595178
INT11	-3103.673342	-3102.460035	-3104.619344
TS(INT11-->8)	-3103.656055	-3102.439377	-3104.603678
8	-3103.687851	-3102.473114	-3104.635777
8 triplet	-3103.638676	-3102.429602	-3104.586388

The harmonic oscillator approach may fail for low vibrational frequencies and it can lead to an overestimation of entropic effects in bimolecular processes. For this reason, we have used models of **1**, **2**, **INT1**, **7** and **INT6** in which iPr and tBu groups have been replaced by Me. The difference between Gibbs energy and energy for these systems has been applied to calculate the Gibbs reaction energies for the formation of **INT1** and **INT6**.

Energies and Gibbs energies (in a.u) computed for model systems at the M06-2X/6-31G(d) level of calculation

	E	G
mod-1	-1934.514706	-1934.039226
mod-2	-304.6519698	-304.554043
mod-INT1	-2239.217937	-2238.616298
mod-7	-383.1538097	-383.008254
mod-INT6	-2317.729919	-2317.078236

Cartesian coordinates (in Å) for all the computed structures

1

P	-1.515706	-0.252629	0.140922
Si	-4.070150	-0.047363	0.101673
N	1.477457	-0.450816	0.175059
N	-2.752577	0.210618	1.240366
N	-2.781418	-0.535720	-0.977078
C	-0.610568	-1.672793	0.572822
C	0.774238	-1.550172	0.513809
C	1.346936	-2.871188	0.992202
H	2.389027	-3.055234	0.727633
C	1.045924	-2.901275	2.524202
H	1.592578	-3.723124	2.995384
H	1.357158	-1.970773	3.009089
C	-0.492831	-3.125669	2.585866
H	-0.727829	-4.104493	3.017641
H	-1.011373	-2.366137	3.173402
C	-0.901545	-3.073373	1.090314
H	-1.905189	-3.451533	0.881245
C	0.278056	-3.846374	0.460733
H	0.238331	-3.879152	-0.632805
H	0.398273	-4.859729	0.860064
C	-5.278896	-1.389871	0.597483
H	-5.922488	-1.679684	-0.241148
H	-5.931052	-1.049624	1.409833
H	-4.739975	-2.277818	0.941592
C	-5.012512	1.476678	-0.445708
H	-4.323850	2.236864	-0.826566
H	-5.593700	1.915416	0.373206
H	-5.717014	1.223282	-1.246048
C	-2.597844	1.123359	2.382136
C	-3.840807	0.956695	3.260427
H	-4.747272	1.235406	2.707685
H	-3.780353	1.602525	4.142139
H	-3.940185	-0.082831	3.588273
C	-1.352633	0.740330	3.187960
H	-1.418374	-0.296360	3.529680
H	-1.254333	1.393547	4.060828
H	-0.439832	0.851576	2.588644
C	-2.477839	2.580429	1.915585
H	-1.613430	2.702260	1.253119
H	-2.349626	3.252238	2.771620
H	-3.378835	2.886628	1.373641

C	-2.696426	-1.198190	-2.280009
C	-2.770752	-2.721259	-2.109878
H	-1.922177	-3.075938	-1.516037
H	-2.750141	-3.227072	-3.081627
H	-3.695633	-3.001295	-1.592870
C	-1.383304	-0.818898	-2.973117
H	-1.286713	0.268077	-3.069832
H	-1.338455	-1.268760	-3.970588
H	-0.521158	-1.188446	-2.402762
C	-3.879983	-0.711365	-3.120249
H	-4.831424	-0.975962	-2.640283
H	-3.868477	-1.176874	-4.110787
H	-3.841233	0.375922	-3.241073
C	2.897920	-0.526732	0.026760
C	3.725579	0.068689	0.994082
C	5.109425	0.035226	0.800422
H	5.760409	0.500313	1.536269
C	5.663037	-0.583493	-0.310918
H	6.740153	-0.601759	-0.445654
C	4.832843	-1.183009	-1.252541
H	5.273140	-1.665564	-2.120042
C	3.446108	-1.164536	-1.106221
C	3.159521	0.745697	2.229622
H	2.078699	0.569660	2.240371
C	3.742371	0.150184	3.516673
H	3.600773	-0.934647	3.553268
H	3.257944	0.592513	4.393470
H	4.816432	0.349876	3.596580
C	3.390575	2.260460	2.174698
H	4.462653	2.489065	2.183529
H	2.932328	2.751303	3.040486
H	2.955711	2.686468	1.265217
C	2.553439	-1.769163	-2.179132
H	1.586534	-2.010704	-1.724854
C	3.109337	-3.071987	-2.760556
H	4.011021	-2.899453	-3.357309
H	2.367135	-3.530421	-3.421880
H	3.356475	-3.789113	-1.970889
C	2.298745	-0.740816	-3.290697
H	1.836628	0.169347	-2.891725
H	1.637346	-1.158121	-4.058731
H	3.244875	-0.460527	-3.767768
C	0.685772	2.942943	-0.261840
C	0.725374	2.487749	-1.548677

Al	0.456700	1.067352	-0.335965
C	0.851976	3.218277	-2.860956
C	-0.391676	4.071344	-3.135280
H	0.984712	2.503136	-3.681259
H	1.743205	3.859166	-2.861255
H	-0.320550	4.592167	-4.095536
H	-1.288307	3.442291	-3.151839
H	-0.530441	4.820013	-2.347885
C	0.804581	4.325283	0.329379
C	1.817566	5.242341	-0.363285
H	1.063583	4.242713	1.392152
H	-0.189561	4.796745	0.307401
H	1.937043	6.181303	0.186904
H	2.797275	4.756579	-0.424250
H	1.505656	5.489971	-1.381852

2

N	-0.173491	6.947591	-0.299558
N	-1.965602	6.083451	-1.045385
C	-0.707232	5.739664	-0.644127
C	-1.061164	8.008499	-0.482871
C	-2.213135	7.453458	-0.950861
C	-0.772829	9.444872	-0.184261
H	-1.563582	10.075322	-0.597067
H	0.170645	9.777390	-0.627397
H	-0.720729	9.639796	0.892095
C	-3.490012	8.134271	-1.327099
H	-3.476666	9.168151	-0.974847
H	-4.363269	7.650947	-0.878889
H	-3.642264	8.154888	-2.411376
C	1.231153	7.018330	0.108922
H	1.484371	5.968617	0.277429
C	2.111145	7.545051	-1.023551
H	1.959152	6.943926	-1.923667
H	3.166553	7.490806	-0.738505
H	1.880788	8.588547	-1.261079
C	1.441905	7.782137	1.415240
H	1.370426	8.864427	1.277573
H	2.442640	7.567303	1.801889
H	0.709599	7.474133	2.166929
C	-2.910570	5.028364	-1.417850
H	-2.264474	4.152373	-1.515870

C	-3.594286	5.277412	-2.761271
H	-4.381042	6.033379	-2.691007
H	-4.061854	4.350235	-3.105997
H	-2.866858	5.595788	-3.513376
C	-3.910971	4.759461	-0.294814
H	-3.378133	4.545126	0.635137
H	-4.539321	3.899254	-0.546389
H	-4.568911	5.618108	-0.126865

INT1

P	2.011685	-0.195952	-0.130909
Si	4.219357	1.112800	0.070889
N	-0.717289	-1.247663	-0.559538
N	3.399220	-0.184923	0.903948
N	2.918551	0.951112	-1.101786
N	-1.544421	2.768166	-0.522912
N	-3.017914	1.643117	0.565118
C	0.306371	-2.042876	-0.915397
C	5.981892	0.761365	-0.484012
H	6.312920	1.477530	-1.245054
H	6.665838	0.857187	0.366499
H	6.083049	-0.248338	-0.891367
C	4.200578	2.768281	0.951699
H	3.195551	2.959110	1.343456
H	4.908052	2.798309	1.788212
H	4.463567	3.582708	0.266021
C	3.620834	-0.819165	2.210281
C	5.127357	-1.073013	2.338383
H	5.683590	-0.126893	2.352141
H	5.347080	-1.596678	3.274445
H	5.490169	-1.677643	1.500718
C	2.879916	-2.156278	2.266925
H	3.227413	-2.823144	1.470565
H	3.054162	-2.640370	3.234097
H	1.801108	-2.007492	2.151261
C	3.162340	0.083155	3.360469
H	2.085471	0.252978	3.293424
H	3.390168	-0.378797	4.328962
H	3.673472	1.052384	3.315411
C	2.985338	1.034421	-2.567021
C	4.034562	0.058610	-3.130863
H	3.919086	-0.925787	-2.668648
H	3.932010	-0.050133	-4.216735

H	5.049105	0.411583	-2.925774
C	1.625568	0.719235	-3.203986
H	0.843843	1.380195	-2.821797
H	1.682803	0.856692	-4.289246
H	1.322395	-0.312642	-3.001980
C	3.400526	2.466373	-2.921625
H	4.391467	2.692578	-2.507797
H	3.451572	2.606404	-4.007121
H	2.691789	3.184228	-2.498571
C	-2.036920	-1.709434	-0.849097
C	-2.659042	-2.701109	-0.053108
C	-3.892645	-3.216487	-0.460159
H	-4.360755	-3.997916	0.133637
C	-4.527033	-2.759208	-1.607842
H	-5.475368	-3.186987	-1.918419
C	-3.947725	-1.730451	-2.338809
H	-4.457759	-1.348912	-3.219866
C	-2.719548	-1.175912	-1.966883
C	-2.048238	-3.212129	1.245741
H	-1.152338	-2.616121	1.451266
C	-1.662763	-4.697343	1.192972
H	-0.909218	-4.911219	0.432939
H	-1.258965	-5.010147	2.162288
H	-2.541657	-5.318145	0.982666
C	-3.026236	-3.013433	2.413107
H	-3.908480	-3.654266	2.300297
H	-2.542901	-3.273679	3.360890
H	-3.369330	-1.977457	2.483580
C	-2.174112	-0.006589	-2.775757
H	-1.307655	0.390728	-2.236566
C	-1.709192	-0.424412	-4.174053
H	-2.536880	-0.856436	-4.748311
H	-1.330884	0.444182	-4.726051
H	-0.909701	-1.166073	-4.125555
C	-3.225583	1.105129	-2.899596
H	-3.627619	1.391543	-1.923665
H	-2.793770	1.996828	-3.367860
H	-4.063645	0.785778	-3.529019
C	-1.746759	1.584722	0.103802
C	-2.673284	3.576474	-0.440272
C	-3.609598	2.860785	0.243742
C	-2.812816	4.931930	-1.052562
H	-3.704706	5.421134	-0.656362
H	-1.959119	5.575765	-0.826286

H	-2.918896	4.878973	-2.141096
C	-5.035247	3.221472	0.508821
H	-5.180285	4.291191	0.345252
H	-5.713917	2.687781	-0.164831
H	-5.338856	3.001590	1.533996
C	-0.220744	3.143443	-1.048914
H	0.340720	2.203299	-1.063813
C	0.509144	4.076180	-0.087570
H	0.570871	3.606842	0.898137
H	1.526383	4.247880	-0.454719
H	0.007034	5.045046	0.002018
C	-0.295573	3.681709	-2.475640
H	-0.704886	4.693124	-2.516033
H	0.711069	3.722369	-2.898721
H	-0.900526	3.027976	-3.111752
C	-3.603369	0.574812	1.397181
H	-2.850029	-0.217261	1.368260
C	-3.735401	1.027096	2.849327
H	-4.477848	1.821149	2.969837
H	-4.055204	0.178479	3.462805
H	-2.767487	1.376598	3.219677
C	-4.895733	0.019106	0.807908
H	-4.775548	-0.194327	-0.258563
H	-5.134822	-0.924352	1.308405
H	-5.743513	0.694924	0.951704
C	-0.472149	-0.007506	2.672544
C	0.054295	1.222828	2.440030
Al	-0.287531	0.241973	0.765983
C	0.441768	2.369026	3.343677
C	0.362216	2.184289	4.863492
H	1.472149	2.660034	3.084057
H	-0.168628	3.242357	3.063143
H	0.764640	3.060481	5.384546
H	0.937224	1.308534	5.184093
H	-0.671318	2.045574	5.195601
C	-0.900909	-0.711416	3.943816
C	-0.078756	-1.964442	4.256111
H	-0.865361	-0.047902	4.815738
H	-1.951710	-1.013032	3.841498
H	-0.469599	-2.488751	5.135559
H	0.966431	-1.703491	4.454822
H	-0.086788	-2.662518	3.410536
C	1.672154	-1.743667	-0.831289
C	0.226375	-3.452802	-1.493573

H	-0.734860	-3.950428	-1.377612
C	0.716487	-3.401117	-2.967324
H	0.513786	-4.360959	-3.451867
H	0.198404	-2.630898	-3.540811
C	2.240113	-3.135369	-2.842242
H	2.820379	-3.986198	-3.216147
H	2.551257	-2.251257	-3.400194
C	2.425731	-2.977204	-1.307879
H	3.462850	-3.042435	-0.967063
C	1.462382	-4.079317	-0.809783
H	1.694908	-5.078825	-1.197397
H	1.382176	-4.106937	0.281168

TS(INT1-->INT2)

Al	0.471848	-0.351433	0.535076
P	-1.965408	0.325228	0.082794
Si	-4.391854	-0.339066	-0.480406
N	0.817961	1.531201	0.073469
N	-3.423534	-0.008461	0.940456
N	2.460693	-1.977474	-1.130439
N	0.509164	-2.965501	-1.024528
C	-1.577344	2.012914	0.290583
C	-0.238540	2.363535	0.228007
C	-0.194600	3.875229	0.400723
H	0.789326	4.292550	0.617431
C	-0.897101	4.513664	-0.839939
H	-0.709667	5.591542	-0.856978
H	-0.518321	4.100069	-1.778178
C	-2.403201	4.197884	-0.618422
H	-2.964982	5.112477	-0.398665
H	-2.873122	3.717202	-1.477583
C	-2.359871	3.276785	0.623791
H	-3.330788	3.096649	1.093896
C	-1.302337	4.025008	1.468873
H	-1.559647	5.072019	1.668716
H	-1.060470	3.511282	2.404473
C	-5.752727	0.909311	-0.807852
H	-6.575176	0.799717	-0.092078
H	-6.172830	0.792406	-1.813687
H	-5.354380	1.925400	-0.718526
C	-5.094818	-2.073963	-0.606740
H	-4.323144	-2.815887	-0.378281
H	-5.474152	-2.273039	-1.615456

H	-5.926774	-2.222712	0.091365
N	-2.893344	-0.068613	-1.332218
C	-2.506893	0.100274	-2.731461
C	-1.039020	-0.289784	-2.910892
H	-0.392563	0.346474	-2.293062
H	-0.734567	-0.156971	-3.954600
H	-0.855933	-1.329126	-2.623863
C	-3.397313	-0.818468	-3.572299
H	-3.286751	-1.858200	-3.247459
H	-3.132020	-0.750698	-4.632216
H	-4.452980	-0.532416	-3.474904
C	-2.689368	1.554134	-3.185003
H	-3.714140	1.892442	-2.993444
H	-2.481216	1.659783	-4.255846
H	-2.000854	2.203701	-2.634306
C	-3.574198	-0.337528	2.358210
C	-2.623744	0.521838	3.196563
H	-1.578753	0.322767	2.929558
H	-2.749378	0.296015	4.261232
H	-2.824973	1.586251	3.034708
C	-3.275137	-1.823539	2.585113
H	-3.967487	-2.445006	2.005898
H	-3.372122	-2.096314	3.642194
H	-2.252170	-2.049318	2.263319
C	-5.022826	-0.030288	2.748131
H	-5.249219	1.025813	2.568723
H	-5.194322	-0.254060	3.805883
H	-5.722733	-0.640485	2.162237
C	2.117888	2.111285	-0.069023
C	2.562474	2.476623	-1.359143
C	3.879501	2.909113	-1.522446
H	4.235994	3.168825	-2.516098
C	4.738591	3.019021	-0.435010
H	5.761329	3.354539	-0.577273
C	4.267960	2.729822	0.838711
H	4.926631	2.864592	1.692369
C	2.960543	2.279910	1.050049
C	1.647800	2.408400	-2.571899
H	0.623233	2.271741	-2.212100
C	1.686980	3.707741	-3.386421
H	1.543291	4.585449	-2.748746
H	0.897870	3.698887	-4.146217
H	2.642808	3.825107	-3.908277
C	1.986824	1.212871	-3.467876

H	1.337970	1.200900	-4.350883
H	1.855521	0.262678	-2.938029
H	3.026132	1.275202	-3.810980
C	2.472280	2.078363	2.477016
H	1.496398	1.584436	2.438102
C	2.294411	3.435641	3.174012
H	1.910745	3.291397	4.189782
H	1.594554	4.080883	2.635253
H	3.252299	3.963820	3.245740
C	3.413042	1.195196	3.301535
H	3.503135	0.198344	2.861432
H	3.025191	1.083731	4.318969
H	4.414512	1.632610	3.376712
C	1.177268	-1.809338	-0.619060
C	2.646567	-3.312807	-1.524364
C	1.446243	-3.928375	-1.450927
C	3.955325	-3.880454	-1.964458
H	4.753012	-3.660863	-1.247099
H	4.272029	-3.499333	-2.940772
H	3.877704	-4.966651	-2.043616
C	1.104789	-5.326267	-1.850270
H	0.526981	-5.362178	-2.780495
H	0.529716	-5.853445	-1.083015
H	2.023139	-5.893584	-2.014777
C	3.495059	-0.953441	-1.001812
H	2.935571	-0.017476	-0.926717
C	4.348645	-1.080660	0.262829
H	3.721606	-1.087864	1.155727
H	5.027629	-0.223026	0.323709
H	4.948047	-1.997787	0.248038
C	4.391110	-0.837629	-2.240122
H	5.220282	-1.549751	-2.210145
H	4.820230	0.169433	-2.265146
H	3.825377	-0.995266	-3.162152
C	-0.881785	-3.233435	-0.672709
H	-1.328293	-2.242192	-0.532284
C	-1.658624	-3.905491	-1.811606
H	-1.373640	-3.492740	-2.784046
H	-2.730283	-3.735276	-1.668024
H	-1.501325	-4.986828	-1.834553
C	-1.034870	-4.017889	0.634767
H	-2.098105	-4.172312	0.850840
H	-0.583367	-3.476864	1.469700
H	-0.559921	-5.001388	0.558891

C	0.826063	-0.993970	2.299968
C	1.443115	-1.970330	1.589728
C	0.784829	-0.819817	3.809371
H	1.797267	-0.890732	4.223659
H	0.417009	0.181528	4.074793
C	-0.095231	-1.870057	4.494098
H	-1.144297	-1.744026	4.215112
H	-0.025261	-1.802445	5.585131
H	0.204046	-2.880486	4.193232
C	2.288272	-3.154161	1.994659
H	1.634246	-4.039807	2.025596
H	2.995408	-3.361127	1.178764
C	3.087133	-3.063610	3.303080
H	3.711908	-2.162992	3.315899
H	3.750607	-3.929063	3.410932
H	2.438871	-3.029430	4.182781

INT2

Al	-0.558464	0.285557	0.422775
P	1.866661	-0.420129	0.170174
Si	4.342814	-0.060964	-0.429165
N	-0.945422	-1.590991	0.181859
N	3.322005	-0.024828	0.998082
N	-2.381386	2.579359	-0.862253
N	-0.070537	2.800656	-0.946984
C	1.417778	-2.052132	0.622922
C	0.089599	-2.411614	0.505627
C	0.022894	-3.900473	0.807440
H	-0.973351	-4.293039	1.017933
C	0.774447	-4.636260	-0.349317
H	0.601764	-5.714072	-0.272655
H	0.422738	-4.316430	-1.332614
C	2.269118	-4.278761	-0.109997
H	2.845541	-5.168247	0.167054
H	2.745453	-3.827546	-0.983203
C	2.180241	-3.287677	1.075962
H	3.132666	-3.078704	1.571248
C	1.087225	-3.974947	1.925359
H	1.333482	-5.006052	2.204812
H	0.811922	-3.399010	2.813998
C	5.526133	-1.514817	-0.485661
H	6.351437	-1.392116	0.224746

H	5.964479	-1.627775	-1.484366
H	4.994155	-2.439950	-0.240264
C	5.305850	1.494443	-0.842669
H	4.669334	2.381747	-0.882543
H	5.804315	1.386997	-1.812624
H	6.090448	1.667853	-0.096730
N	2.827844	-0.325698	-1.258570
C	2.371691	-0.467404	-2.640337
C	0.925079	0.020601	-2.738467
H	0.253097	-0.663016	-2.202715
H	0.592486	0.051148	-3.781910
H	0.824547	1.017227	-2.295019
C	3.271305	0.406772	-3.517754
H	3.222776	1.450358	-3.186905
H	2.961705	0.352663	-4.566397
H	4.315412	0.072011	-3.460423
C	2.453030	-1.929776	-3.093579
H	3.476143	-2.310608	-2.993233
H	2.141658	-2.035454	-4.139361
H	1.793690	-2.547493	-2.473126
C	3.474426	0.505470	2.351433
C	2.497309	-0.196955	3.297517
H	1.461302	-0.021796	2.985610
H	2.611445	0.185771	4.317601
H	2.675507	-1.277488	3.301524
C	3.213089	2.016532	2.345756
H	3.919274	2.520069	1.675605
H	3.317217	2.447092	3.348377
H	2.196647	2.217155	1.984300
C	4.910379	0.222212	2.800741
H	5.105990	-0.855150	2.790492
H	5.079755	0.601363	3.813507
H	5.632217	0.714406	2.136867
C	-2.254581	-2.149319	0.026408
C	-2.642306	-2.672723	-1.226318
C	-3.954875	-3.114919	-1.394011
H	-4.266073	-3.500767	-2.361257
C	-4.869426	-3.071248	-0.348742
H	-5.887238	-3.418708	-0.497019
C	-4.464774	-2.598760	0.891737
H	-5.170198	-2.597207	1.718569
C	-3.162653	-2.135019	1.103874
C	-1.681286	-2.769046	-2.400638
H	-0.674096	-2.559250	-2.026948

C	-1.673992	-4.180099	-3.005294
H	-1.564018	-4.948659	-2.234257
H	-0.847332	-4.281452	-3.717125
H	-2.602368	-4.383488	-3.549747
C	-2.000289	-1.739917	-3.493344
H	-1.321520	-1.871232	-4.344092
H	-1.895839	-0.711852	-3.135172
H	-3.027721	-1.870144	-3.852954
C	-2.761044	-1.700160	2.504396
H	-1.752301	-1.278332	2.459730
C	-2.716594	-2.910920	3.446727
H	-2.381240	-2.606024	4.443824
H	-2.031041	-3.679065	3.074900
H	-3.708506	-3.365904	3.547202
C	-3.695158	-0.621033	3.060769
H	-3.655567	0.286671	2.448599
H	-3.402264	-0.356524	4.081754
H	-4.733534	-0.967168	3.094242
C	-1.159947	2.121858	-0.181308
C	-1.987551	2.931576	-2.172386
C	-0.653591	3.104834	-2.217586
C	-2.977427	3.223670	-3.253444
H	-3.606015	4.076708	-2.972858
H	-3.643180	2.381778	-3.463894
H	-2.463430	3.481434	-4.181131
C	0.194099	3.525235	-3.374510
H	1.024032	2.823366	-3.524016
H	0.637600	4.519415	-3.243206
H	-0.390543	3.550438	-4.296952
C	-3.606151	1.850053	-0.543571
H	-3.479151	1.577088	0.512194
C	-4.847166	2.740000	-0.612074
H	-4.682957	3.665731	-0.052248
H	-5.705736	2.214655	-0.180153
H	-5.105821	2.999811	-1.642607
C	-3.791727	0.545419	-1.323102
H	-4.163647	0.722738	-2.337472
H	-4.497557	-0.122465	-0.816506
H	-2.838333	0.018649	-1.399950
C	0.766054	3.819603	-0.295490
H	0.732717	3.578475	0.773097
C	2.221994	3.645236	-0.732627
H	2.509842	2.596262	-0.600232
H	2.890544	4.277746	-0.136108

H	2.361776	3.906901	-1.787327
C	0.292172	5.269088	-0.466034
H	0.480684	5.636603	-1.479316
H	0.827446	5.926513	0.227720
H	-0.779181	5.357472	-0.271824
C	-0.871563	1.309566	2.077677
C	-1.229347	2.393998	1.339406
C	-0.870667	1.235201	3.587033
H	-1.900104	1.334035	3.952929
H	-0.544954	0.237982	3.911812
C	0.002183	2.282655	4.286448
H	1.046400	2.189400	3.977740
H	-0.040565	2.162795	5.374076
H	-0.321399	3.299754	4.046581
C	-1.781972	3.735957	1.795443
H	-0.974843	4.373662	2.182776
H	-2.172779	4.235758	0.902820
C	-2.915184	3.655273	2.823922
H	-3.681819	2.941877	2.500701
H	-3.394669	4.632860	2.935912
H	-2.566486	3.345826	3.812246

TS(INT2-->INT3)

Al	0.553708	-0.502475	0.261072
P	-2.141514	-0.038860	0.114873
Si	-4.605419	-0.592929	-0.475669
N	0.535866	1.427775	0.242197
N	-3.558060	-0.633342	0.920755
N	3.275690	-1.671517	-0.958094
N	0.730637	-2.047720	-0.980883
C	-1.870488	1.597879	0.663032
C	-0.592089	2.104926	0.581442
C	-0.712542	3.603672	0.829257
H	0.211735	4.120598	1.090741
C	-1.435414	4.188597	-0.426817
H	-1.416063	5.281998	-0.383441
H	-0.943441	3.889401	-1.356315
C	-2.887032	3.641766	-0.304556
H	-3.605384	4.458897	-0.175226
H	-3.196919	3.052444	-1.171652
C	-2.799696	2.758307	0.967352
H	-3.763947	2.474824	1.398308
C	-1.870884	3.619640	1.847328

H	-2.254730	4.629889	2.031533
H	-1.616673	3.134750	2.794186
C	-6.016737	0.642537	-0.395850
H	-6.525154	0.725427	-1.363144
H	-5.633377	1.632573	-0.128545
H	-6.768066	0.352900	0.347043
C	-5.288903	-2.250338	-1.033709
H	-4.492759	-2.998816	-1.101328
H	-5.771461	-2.169989	-2.014820
H	-6.047150	-2.616761	-0.331401
N	-3.175406	-0.020763	-1.292196
C	-2.824017	0.153496	-2.699616
C	-1.496066	0.905173	-2.815461
H	-1.562829	1.878056	-2.317148
H	-1.236471	1.067292	-3.867681
H	-0.676002	0.336806	-2.354363
C	-2.709696	-1.215259	-3.379774
H	-1.972304	-1.822276	-2.851249
H	-2.403494	-1.121190	-4.428503
H	-3.671284	-1.739735	-3.348208
C	-3.933277	0.963266	-3.381124
H	-4.891861	0.433092	-3.315379
H	-3.708626	1.111367	-4.442834
H	-4.050479	1.941425	-2.905111
C	-3.697996	-1.174414	2.270275
C	-2.577166	-0.635437	3.160715
H	-1.595841	-0.872644	2.736306
H	-2.632780	-1.082915	4.159031
H	-2.647333	0.453573	3.252187
C	-3.658808	-2.708386	2.214270
H	-4.531319	-3.089361	1.671519
H	-3.656095	-3.151450	3.216721
H	-2.765773	-3.042788	1.678767
C	-5.051534	-0.725655	2.832082
H	-5.113726	0.367079	2.849463
H	-5.193701	-1.105733	3.849367
H	-5.874838	-1.109767	2.216283
C	1.777159	2.146214	0.315763
C	2.299552	2.752893	-0.845341
C	3.524680	3.418513	-0.771914
H	3.937166	3.873672	-1.668590
C	4.217901	3.516934	0.427576
H	5.168944	4.039136	0.469992
C	3.675066	2.956167	1.576067

H	4.203099	3.056414	2.520795
C	2.457499	2.269684	1.546470
C	1.554862	2.708926	-2.166271
H	0.537272	2.378232	-1.949313
C	1.473279	4.083117	-2.839146
H	1.105610	4.847535	-2.147055
H	0.794319	4.039910	-3.698015
H	2.450332	4.409450	-3.211714
C	2.177281	1.675232	-3.108009
H	1.626873	1.627903	-4.055751
H	2.158096	0.682690	-2.647427
H	3.220039	1.933856	-3.332547
C	1.890021	1.738524	2.853624
H	1.024743	1.109442	2.622622
C	1.416839	2.892024	3.749035
H	0.981552	2.502047	4.675685
H	0.664055	3.509337	3.250913
H	2.258035	3.541268	4.018232
C	2.908426	0.876010	3.606575
H	3.326592	0.110172	2.949430
H	2.428180	0.376560	4.455888
H	3.731079	1.482533	4.002319
C	2.301515	-1.334833	-0.003609
C	2.712331	-1.678349	-2.235913
C	1.378396	-1.932417	-2.256667
C	3.550800	-1.501513	-3.470104
H	4.121185	-2.405683	-3.710922
H	4.260307	-0.677819	-3.359315
H	2.916076	-1.262528	-4.324444
C	0.616550	-2.217855	-3.523095
H	0.094415	-1.330307	-3.904066
H	-0.146576	-2.980413	-3.347847
H	1.266845	-2.593766	-4.317126
C	4.664191	-1.350286	-0.615762
H	4.740066	-1.612730	0.442198
C	5.696346	-2.209165	-1.348200
H	5.372935	-3.254222	-1.380024
H	6.648055	-2.158229	-0.810362
H	5.882147	-1.868057	-2.368734
C	4.950543	0.152118	-0.710041
H	4.853900	0.523035	-1.735843
H	5.967511	0.369179	-0.365046
H	4.244629	0.708296	-0.085174
C	0.227677	-3.381142	-0.596892

H	0.318277	-3.374554	0.500836
C	-1.257549	-3.619460	-0.894646
H	-1.859770	-2.748756	-0.611425
H	-1.615596	-4.482476	-0.320424
H	-1.440485	-3.831591	-1.953316
C	1.107831	-4.518814	-1.114766
H	1.014560	-4.646520	-2.198549
H	0.817207	-5.461311	-0.639317
H	2.158933	-4.317086	-0.883694
C	1.141315	-1.476651	1.965697
C	2.280098	-1.921926	1.357424
C	0.748200	-1.960367	3.337845
H	1.641071	-2.174247	3.940530
H	0.202087	-1.173850	3.874122
C	-0.118922	-3.225131	3.293581
H	-0.994909	-3.071186	2.659399
H	-0.467043	-3.506836	4.292890
H	0.442398	-4.068105	2.876989
C	3.225583	-2.997920	1.871219
H	2.641065	-3.797813	2.342762
H	3.730335	-3.459638	1.012449
C	4.273609	-2.511753	2.881864
H	4.900683	-1.714201	2.469758
H	4.930308	-3.333548	3.184210
H	3.798413	-2.110357	3.781548

INT3

Al	-1.113979	-0.394127	0.453062
P	2.505361	-0.518020	0.214410
Si	5.108049	-0.607116	0.306524
N	-0.436140	1.033164	-0.573694
N	3.821160	-1.413452	-0.541054
N	-3.902122	-1.312553	0.145897
N	-2.125275	0.095039	1.967364
C	1.965592	0.557020	-1.111728
C	0.761385	1.200748	-1.237738
C	0.974755	2.282975	-2.300767
H	0.069173	2.737915	-2.702227
C	1.983134	3.328778	-1.723406
H	2.028309	4.197924	-2.387913
H	1.683660	3.686218	-0.736976
C	3.331919	2.561033	-1.691920
H	4.055133	3.005766	-2.385867

H	3.788633	2.521350	-0.700366
C	2.900665	1.150998	-2.163612
H	3.725860	0.491476	-2.445083
C	1.894873	1.517021	-3.268966
H	2.315606	2.156505	-4.054558
H	1.414542	0.640345	-3.714127
C	6.378916	0.318175	-0.722881
H	7.053409	-0.363147	-1.253309
H	6.995176	0.955380	-0.077054
H	5.886107	0.961029	-1.458713
C	6.047461	-1.691305	1.527651
H	5.352800	-2.275177	2.139738
H	6.684591	-1.100834	2.196393
H	6.702527	-2.393153	0.996806
N	3.831384	0.381259	0.959115
C	3.697475	1.153801	2.189770
C	3.451484	0.233720	3.395818
H	2.572957	-0.395355	3.217573
H	3.287590	0.809272	4.314280
H	4.313892	-0.424226	3.550045
C	4.997061	1.936681	2.398521
H	5.847304	1.253532	2.518514
H	4.937754	2.555676	3.300131
H	5.192786	2.585355	1.538167
C	2.535075	2.144004	2.045291
H	2.733253	2.856549	1.237108
H	2.376877	2.699896	2.976579
H	1.604184	1.618853	1.799101
C	3.747575	-2.593070	-1.394926
C	2.470562	-2.552283	-2.240801
H	1.575776	-2.507973	-1.608479
H	2.401948	-3.448179	-2.867510
H	2.464748	-1.667486	-2.885728
C	3.784980	-3.878641	-0.554251
H	4.718315	-3.926781	0.017630
H	3.722836	-4.771631	-1.187336
H	2.953646	-3.897327	0.155049
C	4.965497	-2.579846	-2.327056
H	4.979797	-1.664661	-2.927936
H	4.949937	-3.443933	-3.000005
H	5.896736	-2.627121	-1.747804
C	-1.504770	1.951347	-0.880699
C	-1.630466	3.144525	-0.137193
C	-2.750287	3.955504	-0.339110

H	-2.859020	4.866430	0.244472
C	-3.717767	3.621799	-1.277357
H	-4.585788	4.258617	-1.420449
C	-3.547140	2.486455	-2.060294
H	-4.281542	2.256900	-2.827338
C	-2.447336	1.641239	-1.891133
C	-0.552945	3.594435	0.835088
H	0.323525	2.968822	0.654429
C	-0.151523	5.056171	0.600195
H	0.048301	5.256599	-0.456795
H	0.752374	5.291603	1.173230
H	-0.936819	5.744758	0.930940
C	-0.960341	3.387875	2.295803
H	-0.147344	3.691618	2.965311
H	-1.196796	2.337128	2.477508
H	-1.845593	3.987278	2.542482
C	-2.269476	0.475862	-2.857866
H	-1.552542	-0.228100	-2.421447
C	-1.704274	0.964753	-4.201397
H	-1.606209	0.123976	-4.897001
H	-0.724095	1.431160	-4.096175
H	-2.383500	1.698370	-4.651096
C	-3.577699	-0.273816	-3.139217
H	-4.098048	-0.536964	-2.216497
H	-3.369097	-1.193597	-3.695657
H	-4.255528	0.327443	-3.755436
C	-2.648857	-1.467295	-0.212511
C	-4.251922	-0.056582	0.764794
C	-3.431446	0.515056	1.693110
C	-5.532275	0.590357	0.299799
H	-6.422986	0.260533	0.853863
H	-5.702395	0.381118	-0.760774
H	-5.465196	1.676017	0.394525
C	-3.963461	1.742185	2.415193
H	-3.850406	2.628140	1.778491
H	-3.415823	1.935222	3.337521
H	-5.021236	1.635709	2.669393
C	-4.875575	-2.433699	0.265658
H	-4.307585	-3.316078	-0.022454
C	-5.308459	-2.601206	1.718522
H	-4.435581	-2.703041	2.369522
H	-5.927742	-3.498281	1.815329
H	-5.892376	-1.741202	2.059720
C	-6.069501	-2.330852	-0.686536

H	-6.815606	-1.613565	-0.339606
H	-6.553280	-3.310888	-0.745906
H	-5.755200	-2.047253	-1.695639
C	-1.722345	-0.028626	3.367256
H	-1.873355	0.915974	3.913123
C	-2.541525	-1.110675	4.073028
H	-3.612727	-0.889101	4.005047
H	-2.271391	-1.192779	5.131341
H	-2.365050	-2.078892	3.588318
C	-0.231576	-0.336958	3.435542
H	0.006611	-1.270669	2.907828
H	0.102609	-0.442851	4.472352
H	0.349293	0.471375	2.977885
C	-0.661288	-2.346927	0.219216
C	-1.846632	-2.684733	-0.387102
C	0.313530	-3.391022	0.686142
H	0.573426	-4.074851	-0.136099
H	1.242168	-2.904157	0.999451
C	-0.249092	-4.216400	1.852412
H	-0.515555	-3.568564	2.693732
H	0.487347	-4.943981	2.206634
H	-1.151337	-4.759305	1.552744
C	-2.217440	-4.032180	-0.967593
H	-1.298325	-4.615430	-1.093544
H	-2.841541	-4.613268	-0.275385
C	-2.918062	-3.897864	-2.321818
H	-3.837492	-3.307215	-2.240722
H	-3.178524	-4.876478	-2.734784
H	-2.264061	-3.386187	-3.034796

TS(INT3-->6)

Al	-1.055373	-0.188945	0.707032
P	2.294539	-0.372344	-0.001465
Si	4.824150	-0.269263	0.556076
N	-0.644964	1.286817	-0.409730
N	3.794472	-0.892888	-0.709749
N	-2.930399	-2.226810	-0.179673
N	-2.555040	-0.051343	1.802245
C	1.751970	0.968360	-1.030447
C	0.509915	1.555792	-1.086373
C	0.663372	2.776783	-1.994318
H	-0.268717	3.190700	-2.382831
C	1.518256	3.801299	-1.181620

H	1.519637	4.772315	-1.687299
H	1.109906	3.954555	-0.178250
C	2.933388	3.160710	-1.172979
H	3.648823	3.778951	-1.727270
H	3.333582	3.006108	-0.167089
C	2.682981	1.812975	-1.897106
H	3.590196	1.293476	-2.215407
C	1.707410	2.261509	-2.997780
H	2.105459	3.053292	-3.643485
H	1.344945	1.426905	-3.604052
C	6.060510	1.022543	-0.017563
H	6.792700	0.570822	-0.697241
H	6.613711	1.463281	0.818757
H	5.550699	1.827160	-0.557559
C	5.730598	-1.547233	1.592210
H	5.040246	-2.329199	1.924592
H	6.174421	-1.083309	2.481262
H	6.546238	-2.020742	1.033210
N	3.331650	0.315055	1.244214
C	3.003088	1.119358	2.421630
C	2.737201	0.236945	3.651772
H	1.800591	-0.317593	3.538473
H	2.655224	0.848941	4.557203
H	3.551199	-0.483470	3.788818
C	4.201947	2.027260	2.724662
H	5.091267	1.429495	2.963656
H	3.992099	2.667082	3.587860
H	4.434150	2.664479	1.865246
C	1.767720	1.986988	2.167129
H	1.947249	2.722348	1.379803
H	1.478631	2.511123	3.084985
H	0.917452	1.368962	1.855663
C	3.934290	-1.945300	-1.714646
C	2.733867	-1.900074	-2.666343
H	1.794711	-2.063208	-2.121898
H	2.822968	-2.679375	-3.430631
H	2.670323	-0.924535	-3.160379
C	4.023855	-3.324619	-1.047296
H	4.929849	-3.396466	-0.435821
H	4.046271	-4.129723	-1.790312
H	3.162537	-3.478984	-0.389792
C	5.221542	-1.677174	-2.500663
H	5.180942	-0.692502	-2.977039
H	5.371396	-2.438753	-3.273296

H	6.093047	-1.702283	-1.833921
C	-1.872428	1.837890	-0.928499
C	-2.502191	2.896263	-0.243661
C	-3.770536	3.311169	-0.656863
H	-4.263208	4.123824	-0.128486
C	-4.406898	2.708932	-1.733585
H	-5.398308	3.033304	-2.035415
C	-3.747135	1.716814	-2.448826
H	-4.224487	1.284764	-3.324646
C	-2.475850	1.272500	-2.077325
C	-1.794945	3.668951	0.856190
H	-0.863526	3.139145	1.086683
C	-1.440861	5.074837	0.347817
H	-0.893688	5.033644	-0.598525
H	-0.826543	5.609801	1.080658
H	-2.352174	5.660069	0.179473
C	-2.619832	3.774759	2.140959
H	-2.046885	4.287051	2.921930
H	-2.899277	2.786002	2.510152
H	-3.539399	4.348295	1.977650
C	-1.752586	0.291884	-2.994027
H	-0.833575	-0.041861	-2.499502
C	-1.375864	1.007298	-4.303068
H	-0.754501	0.357801	-4.929685
H	-0.831049	1.937359	-4.125276
H	-2.280643	1.255933	-4.869887
C	-2.574605	-0.954559	-3.339999
H	-2.837555	-1.521169	-2.446129
H	-1.993813	-1.606786	-4.001922
H	-3.497616	-0.690906	-3.869164
C	-1.659681	-1.807049	-0.161162
C	-3.942228	-1.242405	0.146725
C	-3.762655	-0.297324	1.111625
C	-5.178331	-1.301008	-0.727088
H	-6.021805	-1.830408	-0.262541
H	-4.947571	-1.808258	-1.665783
H	-5.520750	-0.298796	-0.996544
C	-4.910941	0.624739	1.469442
H	-4.565747	1.662928	1.497967
H	-5.310498	0.377834	2.460830
H	-5.739732	0.561753	0.766626
C	-3.287938	-3.656649	-0.016789
H	-2.332657	-4.181301	-0.055468
C	-3.890753	-3.885092	1.368154

H	-3.230706	-3.480072	2.141738
H	-4.031775	-4.956182	1.544838
H	-4.862771	-3.389512	1.457849
C	-4.177343	-4.237016	-1.120187
H	-5.223661	-3.947135	-0.997278
H	-4.129739	-5.330090	-1.078228
H	-3.843915	-3.918900	-2.113040
C	-2.659521	0.252442	3.224883
H	-3.396844	1.050161	3.402770
C	-3.120932	-0.975020	4.016639
H	-4.066389	-1.356598	3.615409
H	-3.264632	-0.737880	5.076672
H	-2.377529	-1.775496	3.932578
C	-1.318095	0.762055	3.738145
H	-0.534942	0.007679	3.585131
H	-1.361459	0.983159	4.809096
H	-1.020932	1.676366	3.211405
C	0.366865	-1.647040	0.798326
C	-0.408250	-2.453933	-0.113705
C	1.174935	-2.439982	1.814702
H	1.665357	-3.295981	1.330856
H	1.978264	-1.838491	2.246864
C	0.273553	-2.973542	2.933398
H	-0.182126	-2.150362	3.493039
H	0.845636	-3.585608	3.637600
H	-0.538443	-3.584346	2.524084
C	0.013630	-3.805399	-0.654392
H	1.108937	-3.846605	-0.670819
H	-0.296388	-4.634952	0.000209
C	-0.497610	-4.043512	-2.077784
H	-1.589579	-3.988995	-2.129168
H	-0.188916	-5.023196	-2.455579
H	-0.107856	-3.274287	-2.752527

6

Al	0.963595	0.243636	0.711921
P	-2.170420	0.234902	0.004386
Si	-4.633275	0.121165	0.727012
N	0.793502	-1.291514	-0.424176
N	-3.675548	0.822336	-0.562148
N	2.536004	2.481840	-0.289370
N	2.449637	0.286435	1.815201
C	-1.562448	-0.955263	-1.110078

C	-0.311498	-1.548492	-1.147267
C	-0.436193	-2.724725	-2.111989
H	0.509642	-3.111956	-2.491583
C	-1.296646	-3.787847	-1.360059
H	-1.278445	-4.734533	-1.908789
H	-0.904541	-3.981461	-0.357737
C	-2.717660	-3.160966	-1.351705
H	-3.417585	-3.762556	-1.942294
H	-3.136911	-3.050372	-0.347200
C	-2.468562	-1.783471	-2.018190
H	-3.379474	-1.274334	-2.339754
C	-1.461822	-2.174420	-3.115328
H	-1.838486	-2.941358	-3.801635
H	-1.091469	-1.312442	-3.677393
C	-5.857405	-1.185752	0.168310
H	-6.685590	-0.734223	-0.387909
H	-6.289498	-1.723743	1.018103
H	-5.366260	-1.913466	-0.486588
C	-5.484002	1.340011	1.867042
H	-4.800268	2.152740	2.131776
H	-5.812564	0.851580	2.791855
H	-6.372928	1.775506	1.396609
N	-3.079738	-0.470569	1.285906
C	-2.708557	-1.347664	2.408756
C	-2.363787	-0.531434	3.660989
H	-1.461034	0.062990	3.502058
H	-2.186190	-1.196223	4.513559
H	-3.184781	0.148904	3.914539
C	-3.914041	-2.240086	2.727949
H	-4.779316	-1.639501	3.037365
H	-3.673789	-2.917571	3.553130
H	-4.197545	-2.839746	1.856860
C	-1.523090	-2.244458	2.050008
H	-1.776291	-2.931839	1.240276
H	-1.219117	-2.828990	2.925353
H	-0.660068	-1.654670	1.728673
C	-4.018604	1.678951	-1.705606
C	-2.867563	1.701061	-2.716899
H	-1.909435	1.929909	-2.242157
H	-3.059830	2.458577	-3.483644
H	-2.766392	0.728911	-3.209609
C	-4.355941	3.090696	-1.204518
H	-5.236104	3.054839	-0.552344
H	-4.579881	3.761755	-2.040742

H	-3.533954	3.515153	-0.625046
C	-5.268308	1.112005	-2.392599
H	-5.109870	0.076079	-2.707763
H	-5.518371	1.710541	-3.274741
H	-6.133151	1.140778	-1.718855
C	2.056241	-1.799395	-0.894481
C	2.716246	-2.804292	-0.160827
C	4.001843	-3.190592	-0.546856
H	4.516426	-3.965436	0.015774
C	4.628776	-2.604119	-1.637297
H	5.634495	-2.902612	-1.917051
C	3.944389	-1.658540	-2.391030
H	4.417440	-1.236781	-3.274210
C	2.651738	-1.248178	-2.054112
C	2.025932	-3.555451	0.963717
H	1.093382	-3.028356	1.191475
C	1.672080	-4.973597	0.490796
H	1.113599	-4.954679	-0.449829
H	1.070684	-5.496866	1.242754
H	2.584531	-5.556755	0.321535
C	2.863482	-3.628049	2.242814
H	2.290910	-4.104357	3.046622
H	3.162335	-2.631939	2.576750
H	3.771801	-4.221572	2.090937
C	1.917332	-0.319881	-3.017755
H	0.949961	-0.046195	-2.583568
C	1.674643	-1.047864	-4.351749
H	1.056088	-0.430706	-5.012715
H	1.178427	-2.013073	-4.221334
H	2.626676	-1.231212	-4.862826
C	2.666362	0.986640	-3.301121
H	2.760886	1.594003	-2.400571
H	2.114653	1.568878	-4.048144
H	3.666941	0.794758	-3.706440
C	1.300882	1.870581	-0.187257
C	3.644743	1.636470	0.094943
C	3.595951	0.674098	1.056828
C	4.889810	1.837062	-0.752428
H	5.739872	2.239169	-0.186239
H	4.675061	2.525157	-1.569901
H	5.213889	0.897257	-1.215530
C	4.833073	-0.164150	1.318131
H	4.555597	-1.220386	1.396871
H	5.323227	0.122668	2.257631

H	5.574973	-0.077435	0.525811
C	2.667871	3.917316	0.049776
H	1.654773	4.317056	-0.019180
C	3.140130	4.097698	1.494297
H	2.535451	3.488074	2.172950
H	3.064701	5.149028	1.792376
H	4.183701	3.783412	1.602972
C	3.543699	4.728194	-0.910553
H	4.608242	4.539884	-0.744568
H	3.370136	5.797361	-0.747637
H	3.309955	4.496013	-1.954361
C	2.691561	-0.056171	3.209137
H	3.510828	-0.786095	3.296248
C	3.105077	1.173672	4.024790
H	3.960183	1.673281	3.557084
H	3.380450	0.897570	5.048987
H	2.281584	1.895235	4.066931
C	1.450799	-0.705322	3.807626
H	0.611081	-0.000913	3.796330
H	1.621667	-1.001366	4.847520
H	1.162689	-1.598996	3.240997
C	-0.883131	1.314914	0.622428
C	-0.006199	2.254788	-0.274749
C	-1.469690	2.181065	1.764242
H	-2.067728	2.992678	1.318705
H	-2.172462	1.609006	2.372809
C	-0.412773	2.811152	2.667081
H	0.218010	2.042512	3.127978
H	-0.878848	3.396927	3.465735
H	0.249101	3.470230	2.097576
C	-0.568964	3.576027	-0.767746
H	-1.654913	3.499695	-0.866984
H	-0.411046	4.388436	-0.039281
C	0.015126	3.976980	-2.125633
H	1.108577	3.976818	-2.104361
H	-0.323606	4.971857	-2.433164
H	-0.281869	3.257462	-2.895612

TS(INT3-->INT4)

Al	-0.472001	-0.335306	0.417256
P	1.959440	0.017897	-0.125816
Si	4.285899	-0.975440	0.392268
N	-0.664830	1.448523	-0.419098

N	3.057885	-1.095462	-0.852853
N	-2.710639	-2.080481	0.156239
N	-1.284200	-0.434177	2.082750
C	1.686561	1.415263	-1.116033
C	0.380850	1.913585	-1.119254
C	0.371833	3.077957	-2.102595
H	-0.619003	3.400724	-2.422387
C	1.252963	4.225599	-1.528213
H	1.137295	5.112181	-2.158996
H	0.968780	4.509521	-0.513542
C	2.696361	3.656728	-1.608783
H	3.312352	4.238602	-2.302825
H	3.192800	3.660713	-0.637994
C	2.461921	2.221708	-2.150309
H	3.359945	1.731138	-2.537180
C	1.332083	2.507102	-3.169609
H	1.603310	3.249456	-3.929545
H	0.942832	1.605272	-3.650744
C	5.941725	-0.257041	-0.133547
H	6.509509	-0.972452	-0.737512
H	6.554773	-0.021353	0.744033
H	5.811876	0.659916	-0.716663
C	4.626394	-2.544756	1.357585
H	3.693891	-3.029302	1.659898
H	5.210002	-2.329793	2.259859
H	5.205088	-3.257354	0.758336
N	3.155819	0.142329	1.128290
C	3.340719	1.205138	2.126717
C	3.831929	0.565430	3.429625
H	3.101742	-0.148567	3.816314
H	4.015572	1.332847	4.189388
H	4.776439	0.033005	3.259592
C	4.397986	2.210070	1.644690
H	5.393007	1.755129	1.624433
H	4.440651	3.081170	2.307798
H	4.159391	2.548491	0.633448
C	2.025730	1.954208	2.364677
H	1.717142	2.481578	1.455615
H	2.159227	2.694682	3.160175
H	1.216172	1.281184	2.665264
C	3.021143	-1.807208	-2.138053
C	1.884166	-1.287145	-3.018375
H	0.923388	-1.339613	-2.493756
H	1.813769	-1.902750	-3.921968

H	2.064415	-0.251253	-3.317529
C	2.845541	-3.310697	-1.901638
H	3.623558	-3.688183	-1.227889
H	2.911542	-3.863306	-2.846052
H	1.873521	-3.502784	-1.447453
C	4.352668	-1.574688	-2.864628
H	4.549855	-0.503674	-2.976508
H	4.329856	-2.033994	-3.858476
H	5.185478	-2.025191	-2.312108
C	-1.908687	2.154937	-0.501454
C	-2.119075	3.268208	0.342799
C	-3.360384	3.905880	0.323327
H	-3.536634	4.751741	0.981546
C	-4.371265	3.479802	-0.528890
H	-5.333972	3.981687	-0.530537
C	-4.127522	2.432542	-1.407055
H	-4.899995	2.144287	-2.114684
C	-2.900537	1.760597	-1.423804
C	-1.020610	3.789931	1.254300
H	-0.069803	3.438545	0.848882
C	-0.967404	5.319990	1.302464
H	-0.973246	5.756098	0.298143
H	-0.055224	5.644209	1.814927
H	-1.814724	5.737299	1.856733
C	-1.135170	3.204517	2.662327
H	-0.326365	3.576384	3.302194
H	-1.077056	2.113862	2.615386
H	-2.092645	3.480581	3.120111
C	-2.642536	0.736439	-2.522552
H	-1.708840	0.211777	-2.294824
C	-2.476213	1.453628	-3.871867
H	-2.234455	0.729084	-4.657329
H	-1.678982	2.201679	-3.843610
H	-3.404318	1.963208	-4.155874
C	-3.752080	-0.314400	-2.633910
H	-3.740265	-0.984944	-1.771909
H	-3.609560	-0.912166	-3.540396
H	-4.744171	0.143726	-2.706990
C	-1.438901	-1.803966	-0.398891
C	-3.342345	-1.076507	0.950901
C	-2.681896	-0.320885	1.862937
C	-4.805436	-0.801640	0.666344
H	-5.430941	-0.907909	1.560611
H	-5.192110	-1.481187	-0.093414

H	-4.948014	0.220529	0.289027
C	-3.448462	0.771989	2.585219
H	-3.663246	1.613852	1.912868
H	-2.873205	1.162485	3.426343
H	-4.405227	0.408762	2.974737
C	-3.224783	-3.458731	0.214328
H	-2.337687	-4.099777	0.148451
C	-3.901329	-3.779312	1.546457
H	-3.270230	-3.477863	2.387021
H	-4.087794	-4.856286	1.614470
H	-4.863204	-3.266499	1.643993
C	-4.132668	-3.827070	-0.967147
H	-5.119165	-3.361948	-0.878943
H	-4.282398	-4.912185	-1.007143
H	-3.693062	-3.504934	-1.915448
C	-0.817288	-0.485824	3.463354
H	-0.719372	0.528817	3.897267
C	-1.758050	-1.280092	4.377265
H	-2.753089	-0.835778	4.452056
H	-1.336072	-1.338880	5.386439
H	-1.872562	-2.299741	3.992528
C	0.559165	-1.151315	3.522161
H	0.455376	-2.234301	3.408595
H	1.038972	-0.956863	4.488156
H	1.230421	-0.799029	2.730733
C	-0.037678	-2.733903	0.022487
C	-0.702876	-2.871717	-1.109131
C	0.724959	-3.605504	0.971765
H	1.302822	-4.363183	0.424796
H	1.445394	-3.005993	1.541801
C	-0.235361	-4.305946	1.942733
H	-0.944400	-3.582354	2.357574
H	0.309676	-4.774691	2.768167
H	-0.809485	-5.082134	1.427599
C	-0.902791	-3.812133	-2.257218
H	0.038727	-4.344241	-2.439057
H	-1.637300	-4.580220	-1.979817
C	-1.370321	-3.105331	-3.529941
H	-2.305352	-2.570654	-3.345085
H	-1.535906	-3.821813	-4.339684
H	-0.634075	-2.370128	-3.866969

INT4

Al	-0.518901	0.532874	-0.385722
P	1.662520	-0.763838	-0.034305
Si	4.255158	-0.803656	-0.078464
N	-1.394497	-0.974588	0.478472
N	2.980572	-0.366788	1.032871
N	-1.238324	3.199875	-0.789061
N	-1.034424	0.693615	-2.145302
C	0.767680	-2.176741	0.492262
C	-0.605323	-2.058779	0.701501
C	-1.066384	-3.422007	1.206712
H	-2.036487	-3.421926	1.705954
C	-0.934412	-4.402544	-0.006187
H	-1.420586	-5.352286	0.237089
H	-1.408394	-4.012296	-0.909349
C	0.601138	-4.574179	-0.172896
H	0.907505	-5.601528	0.051461
H	0.942904	-4.333108	-1.179023
C	1.159343	-3.594878	0.890602
H	2.218305	-3.730116	1.125328
C	0.156607	-3.865520	2.031992
H	0.100942	-4.922951	2.315090
H	0.323421	-3.263250	2.926426
C	5.276973	-2.308406	0.393875
H	5.898089	-2.112262	1.275599
H	5.953046	-2.595554	-0.419329
H	4.629301	-3.162358	0.614893
C	5.421155	0.589223	-0.548763
H	4.883460	1.382791	-1.077300
H	6.235224	0.235841	-1.190331
H	5.874781	1.030331	0.345801
N	2.924578	-1.111925	-1.170960
C	2.862047	-1.330351	-2.619729
C	2.989318	-0.182880	2.486459
C	-2.735051	-0.898898	1.022646
C	-3.843530	-1.525093	0.404699
C	-5.126705	-1.308475	0.921630
H	-5.972574	-1.788511	0.437584
C	-5.343851	-0.495661	2.017502
H	-6.349469	-0.324152	2.388519
C	-4.252129	0.080341	2.652742
H	-4.421580	0.693198	3.530075
C	-2.949962	-0.121956	2.195754
C	-3.759695	-2.471411	-0.782598
C	-1.793087	0.399682	3.039666

H	-1.062242	0.871912	2.370535
C	-0.326351	2.432310	0.101653
C	-0.812476	3.093996	-2.163117
C	-0.733701	1.909760	-2.808043
C	-0.390658	4.410750	-2.758588
H	-1.257056	5.077286	-2.860069
H	0.305217	4.917227	-2.078365
C	-0.236184	1.848717	-4.246457
H	-0.854650	2.449759	-4.921909
H	-0.234378	0.821091	-4.613364
C	-2.663665	2.942314	-0.560284
C	-2.016199	-0.222222	-2.744463
C	1.080648	2.986549	0.149652
C	0.350891	3.219265	1.193764
C	2.341369	3.004803	-0.628632
H	2.596185	1.962291	-0.878074
C	0.167137	3.777078	2.553095
H	-0.000223	2.942581	3.248597
H	2.159272	3.502289	-1.590486
H	-0.756343	4.369832	2.571066
H	-2.916454	1.875607	-0.741148
H	-2.732503	-2.460268	-1.156020
H	-2.684882	-0.505935	-1.924188
C	4.326544	0.457817	2.872190
H	4.362411	0.635302	3.951726
H	5.169801	-0.196858	2.618030
H	4.459280	1.414529	2.357363
C	2.844441	-1.521374	3.219417
H	2.900279	-1.380479	4.304782
H	1.882197	-1.977476	2.978651
H	3.639934	-2.212685	2.918262
C	1.857004	0.759574	2.880251
H	1.994707	1.729990	2.397942
H	0.894846	0.351876	2.550944
H	1.815416	0.893871	3.967541
C	2.144199	-0.166055	-3.300273
H	2.677731	0.772743	-3.108010
H	2.091560	-0.318259	-4.384866
H	1.123342	-0.062086	-2.919501
C	4.297873	-1.417996	-3.146365
H	4.288700	-1.646730	-4.216481
H	4.826718	-0.468851	-3.011259
H	4.855058	-2.214544	-2.638448
C	2.148162	-2.650099	-2.918072

H	2.692718	-3.482392	-2.458964
H	1.135495	-2.635217	-2.508118
H	2.078675	-2.823958	-3.997575
C	-4.124746	-3.907468	-0.372695
H	-3.523936	-4.272200	0.461750
H	-5.176315	-3.956613	-0.069879
H	-3.987699	-4.590769	-1.218410
C	-4.705301	-2.050237	-1.921673
H	-4.440969	-2.570240	-2.849180
H	-5.740543	-2.317958	-1.684798
H	-4.678405	-0.974101	-2.105954
C	-1.125854	-0.778068	3.766072
H	-1.873493	-1.320385	4.356021
H	-0.670826	-1.477461	3.063865
H	-0.342831	-0.425591	4.446416
C	-2.193763	1.437143	4.092780
H	-2.728210	2.291046	3.666090
H	-2.823040	0.989035	4.869580
H	-1.294046	1.811797	4.590795
C	-3.016017	3.265625	0.888428
H	-4.071638	3.050324	1.085370
H	-2.413419	2.669928	1.577819
H	-2.822128	4.326613	1.087038
C	-3.519168	3.788961	-1.499564
H	-3.329198	4.852602	-1.315820
H	-3.296112	3.575506	-2.548823
H	-4.581572	3.590712	-1.325546
C	-1.375976	-1.517182	-3.247380
H	-0.829163	-1.996232	-2.424919
H	-2.131968	-2.224261	-3.611266
H	-0.663898	-1.325981	-4.059124
C	-2.918779	0.413387	-3.805130
H	-2.394220	0.615150	-4.742129
H	-3.744675	-0.266822	-4.035811
H	-3.339771	1.354539	-3.436412
H	0.793113	2.219355	-4.324343
H	0.081386	4.316740	-3.739748
C	3.494234	3.670885	0.118341
H	4.402751	3.702067	-0.490534
H	3.231655	4.695968	0.396492
H	3.718975	3.119120	1.037518
C	1.356662	4.617431	3.014150
H	2.272375	4.016832	3.032244
H	1.520592	5.455295	2.330185

H	1.192162	5.018932	4.018155

TS(INT4-->INT5)

Al	0.868223	0.519933	0.547151
P	-1.846111	-0.412842	0.065500
Si	-4.442869	-0.438417	-0.191350
N	1.272908	-1.118780	-0.304188
N	-3.056169	0.035017	-1.135504
N	2.173824	1.985096	0.579845
N	0.801299	0.612497	2.419706
C	-1.075689	-1.925662	-0.481368
C	0.290952	-2.015733	-0.641736
C	0.579405	-3.416673	-1.173981
H	1.555352	-3.545751	-1.646082
C	0.299199	-4.374787	0.027326
H	0.651583	-5.384160	-0.208692
H	0.814408	-4.047495	0.935305
C	-1.248412	-4.325733	0.164775
H	-1.692863	-5.299426	-0.068540
H	-1.573935	-4.039124	1.164562
C	-1.647559	-3.273629	-0.906756
H	-2.710206	-3.265090	-1.157994
C	-0.670921	-3.669571	-2.032110
H	-0.764353	-4.718085	-2.338735
H	-0.734627	-3.023741	-2.909801
C	-5.450739	-1.902001	-0.813895
H	-6.109607	-1.610502	-1.640059
H	-6.092163	-2.287972	-0.012509
H	-4.813926	-2.721836	-1.156164
C	-5.685696	0.925862	0.175317
H	-5.218616	1.776878	0.679927
H	-6.500841	0.556066	0.806417
H	-6.137436	1.287666	-0.754856
N	-3.254783	-0.788810	1.036731
C	-3.344289	-0.949385	2.491057
C	-2.895438	0.410562	-2.538561
C	2.546167	-1.239109	-0.969506
C	3.641802	-1.864586	-0.335809
C	4.887541	-1.851487	-0.969515
H	5.734830	-2.322864	-0.478073
C	5.060115	-1.262630	-2.214082
H	6.037194	-1.256986	-2.687378
C	3.962825	-0.712367	-2.863568

H	4.085191	-0.289720	-3.857627
C	2.700470	-0.697925	-2.266514
C	3.500266	-2.635411	0.964512
C	1.523527	-0.160159	-3.066355
H	0.645800	-0.152768	-2.413769
C	0.473466	2.187199	-0.359067
C	2.027167	2.598604	1.846339
C	1.286031	1.912632	2.755454
C	2.473156	4.023163	2.047507
H	3.565798	4.110642	2.047684
H	2.098252	4.671637	1.245554
C	0.814097	2.536339	4.056559
H	1.614581	2.680015	4.791405
H	0.053707	1.894038	4.505291
C	3.379839	2.141482	-0.234187
C	1.500048	-0.496082	3.105847
C	-0.366962	3.207414	0.259379
C	0.117219	3.451655	-0.938967
C	-1.340090	3.414487	1.361640
H	-1.197485	2.620591	2.102492
C	0.117930	4.282919	-2.170285
H	-0.022213	3.615819	-3.029349
H	-1.141942	4.371529	1.859402
H	1.109195	4.734546	-2.298794
H	3.220265	1.482647	-1.094667
H	2.487241	-2.463847	1.337468
H	2.449345	-0.697672	2.580370
C	-4.252172	0.905433	-3.050869
H	-4.176515	1.198812	-4.102775
H	-5.013708	0.119013	-2.979974
H	-4.585977	1.773393	-2.472643
C	-2.436076	-0.780287	-3.387563
H	-2.401346	-0.515569	-4.451088
H	-1.437314	-1.095520	-3.075129
H	-3.118601	-1.628221	-3.257612
C	-1.884987	1.551640	-2.671651
H	-2.226525	2.426147	-2.105696
H	-0.905875	1.258914	-2.278166
H	-1.764441	1.836396	-3.724297
C	-2.550346	0.148801	3.206956
H	-2.968780	1.128951	2.943540
H	-2.620401	0.026667	4.294682
H	-1.490612	0.148748	2.926892
C	-4.816059	-0.834310	2.903443

H	-4.921598	-1.058897	3.969544
H	-5.196872	0.176897	2.731622
H	-5.438776	-1.548801	2.349996
C	-2.842919	-2.341381	2.885838
H	-3.472758	-3.108078	2.420828
H	-1.819332	-2.487075	2.537815
H	-2.862639	-2.478808	3.973243
C	3.668802	-4.140434	0.704675
H	2.995984	-4.494110	-0.080837
H	4.695116	-4.363132	0.391272
H	3.462668	-4.712003	1.616614
C	4.502529	-2.196894	2.039959
H	4.278724	-2.698956	2.988108
H	5.526056	-2.468323	1.757906
H	4.478746	-1.118237	2.215314
C	1.229036	-1.098831	-4.244676
H	2.064544	-1.104114	-4.954034
H	1.076487	-2.127364	-3.902615
H	0.330447	-0.774796	-4.781375
C	1.741265	1.269032	-3.574109
H	1.882032	1.970562	-2.746036
H	2.614053	1.332727	-4.233353
H	0.867646	1.594273	-4.151356
C	3.644230	3.541270	-0.805461
H	4.353762	3.461400	-1.636210
H	2.724529	3.989385	-1.189750
H	4.075352	4.223718	-0.068741
C	4.608863	1.616529	0.508277
H	4.810201	2.217215	1.402643
H	4.445614	0.580495	0.816677
H	5.493653	1.647048	-0.136853
C	0.648530	-1.758949	3.053619
H	0.250784	-1.937712	2.047226
H	1.232770	-2.638725	3.351492
H	-0.197369	-1.661999	3.742164
C	1.893153	-0.225431	4.559288
H	1.012267	-0.034332	5.181534
H	2.403680	-1.108668	4.958538
H	2.577193	0.622697	4.644259
H	0.352311	3.516527	3.886162
H	2.119812	4.417254	3.002278
C	-2.775518	3.378119	0.821758
H	-3.494034	3.479786	1.641210
H	-2.949322	4.190792	0.109025

H	-2.963447	2.427022	0.309943
C	-0.960226	5.364391	-2.131752
H	-1.956613	4.913481	-2.096952
H	-0.843368	5.995703	-1.245765
H	-0.906571	6.002051	-3.017843

INT5

P	2.016472	-0.207228	-0.220231
Si	4.547304	-0.121409	0.220147
N	-1.322981	-0.996193	-0.448091
N	3.405837	0.471843	-0.975756
N	3.144944	-0.973239	0.831133
N	-2.232722	1.493087	1.341790
N	-1.708976	2.200407	-1.126726
C	1.055268	-1.279434	-1.196385
C	-0.309808	-1.619847	-1.065938
C	-0.510765	-2.853850	-1.947226
H	-1.406900	-3.430884	-1.715616
C	-0.453386	-2.318045	-3.408723
H	-0.773608	-3.102481	-4.101268
H	-1.112298	-1.457815	-3.551853
C	1.046485	-1.961489	-3.595977
H	1.509529	-2.588910	-4.365108
H	1.186514	-0.917180	-3.878676
C	1.643695	-2.274461	-2.195781
H	2.735529	-2.344705	-2.180967
C	0.854814	-3.550110	-1.842717
H	1.073476	-3.930276	-0.841032
H	0.971725	-4.355604	-2.576677
C	5.960476	-1.159693	-0.443546
H	6.460046	-1.710563	0.361381
H	6.714805	-0.520082	-0.913714
H	5.608576	-1.880329	-1.187755
C	5.217040	1.178859	1.391205
H	4.383761	1.757726	1.804250
H	5.907879	1.868339	0.892885
H	5.759038	0.716517	2.223883
C	3.594972	1.534743	-1.974809
C	2.651621	1.306651	-3.150559
H	2.903461	0.368635	-3.654909
H	2.724745	2.127836	-3.871724
H	1.616140	1.245415	-2.810082
C	3.371206	2.912552	-1.351708

H	2.357311	2.983481	-0.961092
H	3.515696	3.709568	-2.089538
H	4.067098	3.074496	-0.520381
C	5.039363	1.442652	-2.479895
H	5.757747	1.656313	-1.678032
H	5.204879	2.181274	-3.270415
H	5.246902	0.446286	-2.883170
C	3.095751	-2.208782	1.627665
C	3.658266	-3.394001	0.827619
H	3.125698	-3.494444	-0.122645
H	3.541267	-4.326738	1.390636
H	4.722834	-3.262508	0.614015
C	1.662237	-2.540869	2.022965
H	1.159796	-1.687841	2.483356
H	1.650111	-3.377579	2.729471
H	1.093167	-2.831188	1.137784
C	3.961259	-1.992938	2.874226
H	5.003767	-1.793615	2.593349
H	3.956276	-2.886881	3.506354
H	3.601444	-1.142088	3.459723
C	-2.587195	-1.674321	-0.259653
C	-3.680344	-1.406746	-1.108729
C	-4.911961	-2.016185	-0.857284
H	-5.748927	-1.795411	-1.514679
C	-5.084941	-2.884072	0.209511
H	-6.048846	-3.348331	0.393316
C	-4.006642	-3.147683	1.041906
H	-4.132853	-3.826111	1.881202
C	-2.761046	-2.552311	0.834670
C	-3.572929	-0.464896	-2.284534
H	-2.538272	-0.132093	-2.324499
C	-3.915051	-1.165628	-3.605024
H	-3.340579	-2.088573	-3.734752
H	-3.703686	-0.505336	-4.454440
H	-4.978451	-1.426067	-3.649865
C	-4.447333	0.777880	-2.084461
H	-5.511252	0.513653	-2.124464
H	-4.251686	1.506730	-2.881397
H	-4.240059	1.262093	-1.124846
C	-1.629933	-2.916635	1.775668
H	-0.838452	-2.177974	1.630105
C	-1.095544	-4.311236	1.418096
H	-1.902273	-5.048564	1.499700
H	-0.290325	-4.615550	2.094659

H	-0.717521	-4.347891	0.391819
C	-2.026840	-2.890300	3.257175
H	-2.535534	-1.960985	3.529376
H	-1.130242	-2.987708	3.879980
H	-2.690056	-3.723908	3.511993
C	0.837194	0.860565	0.633047
C	-2.876475	2.673065	0.889126
C	-2.587987	3.047259	-0.388561
C	-3.661438	3.505734	1.867694
H	-3.025988	3.803598	2.712642
H	-4.519952	2.975669	2.293645
H	-4.045580	4.420257	1.416849
C	-3.220521	4.222886	-1.084721
H	-3.885119	3.885490	-1.891883
H	-2.490900	4.902043	-1.541430
H	-3.829613	4.814888	-0.403732
C	-2.750452	0.683250	2.434473
H	-2.118611	-0.219490	2.416935
C	-2.577485	1.287364	3.839422
H	-1.610459	1.793796	3.915135
H	-2.622602	0.500159	4.602866
H	-3.360423	2.014153	4.073705
C	-4.195970	0.200094	2.240197
H	-4.912937	1.012997	2.389097
H	-4.440631	-0.589280	2.961948
H	-4.339026	-0.200245	1.233394
C	-1.323323	2.628560	-2.462773
H	-2.179105	3.108716	-2.955570
C	-0.927641	1.440738	-3.349059
H	-0.368547	0.691186	-2.771467
H	-0.290875	1.763728	-4.180566
H	-1.803546	0.947453	-3.777898
C	-0.182071	3.654994	-2.445213
H	-0.414391	4.492395	-1.780426
H	0.019865	4.051789	-3.447835
H	0.731217	3.178750	-2.077912
C	1.157485	1.182768	2.110044
C	1.272957	2.181216	1.301879
Al	-1.095803	0.875192	0.040832
C	1.156256	3.652354	1.085634
C	0.313021	4.312404	2.179491
H	0.672164	3.807984	0.116486
H	2.147601	4.117950	1.029100
H	0.140816	5.366681	1.943877

H	-0.655416	3.806173	2.251387
H	0.814868	4.257065	3.149386
C	1.011720	0.653411	3.486508
C	1.173491	1.730493	4.557627
H	1.750267	-0.137938	3.652726
H	0.025816	0.169448	3.558278
H	1.128896	1.289998	5.557458
H	2.137749	2.237178	4.447130
H	0.385479	2.482814	4.479720

TS(INT5-->4)

P	2.162538	-0.143533	-0.102101
Si	4.757423	-0.388428	-0.031262
N	-1.236847	-1.087924	-0.018684
N	3.520915	-0.088598	-1.227508
N	3.406820	-0.675255	1.031883
N	-2.719818	1.708166	0.291900
N	-1.904292	1.346446	-2.152344
C	1.194164	-1.587844	-0.472765
C	-0.148402	-1.878708	-0.252885
C	-0.293327	-3.386531	-0.493865
H	-1.186904	-3.836029	-0.058097
C	-0.171295	-3.567806	-2.038292
H	-0.429210	-4.596237	-2.311098
H	-0.845149	-2.901495	-2.582701
C	1.326518	-3.260522	-2.311356
H	1.844481	-4.139064	-2.711418
H	1.458455	-2.437597	-3.016313
C	1.853616	-2.899599	-0.897551
H	2.941570	-2.904327	-0.802372
C	1.077418	-3.910814	-0.041105
H	1.266414	-3.786189	1.027835
H	1.245069	-4.955412	-0.329137
C	5.902370	-1.837556	-0.352943
H	6.497851	-2.067553	0.537881
H	6.600955	-1.610513	-1.166064
H	5.337044	-2.732599	-0.626677
C	5.823924	1.093173	0.443772
H	5.206825	1.983450	0.604099
H	6.569670	1.327871	-0.323462
H	6.375242	0.895795	1.371114
C	3.618270	0.653839	-2.486691
C	2.605609	0.098921	-3.483548

H	2.864527	-0.932505	-3.741548
H	2.577135	0.698790	-4.400015
H	1.607999	0.096538	-3.044254
C	3.386230	2.151663	-2.247215
H	2.422919	2.308325	-1.751840
H	3.384466	2.715764	-3.186417
H	4.172617	2.555247	-1.598213
C	5.023733	0.442332	-3.059835
H	5.795075	0.861283	-2.403564
H	5.112033	0.939512	-4.031164
H	5.220373	-0.625754	-3.199427
C	3.341012	-0.627790	2.488705
C	4.534718	-1.414338	3.042409
H	4.515554	-2.443293	2.670600
H	4.508226	-1.433013	4.137074
H	5.484077	-0.953143	2.742746
C	2.053097	-1.301788	2.953010
H	1.178647	-0.836794	2.487016
H	1.944160	-1.238564	4.042345
H	2.055084	-2.354988	2.657345
C	3.416528	0.821808	3.000766
H	4.410332	1.241686	2.815352
H	3.219473	0.880751	4.078086
H	2.690171	1.451273	2.475918
C	-2.449235	-1.707892	0.470621
C	-3.498147	-2.042178	-0.411484
C	-4.668076	-2.611086	0.099046
H	-5.472150	-2.862442	-0.587708
C	-4.822456	-2.853423	1.455523
H	-5.737314	-3.297335	1.835737
C	-3.794253	-2.511423	2.322668
H	-3.912063	-2.692647	3.387428
C	-2.612117	-1.932543	1.856924
C	-3.414757	-1.789426	-1.901096
H	-2.413778	-1.410889	-2.106704
C	-3.624248	-3.074537	-2.711225
H	-2.968656	-3.880968	-2.367900
H	-3.418649	-2.892009	-3.772411
H	-4.658648	-3.427547	-2.633530
C	-4.415550	-0.708820	-2.328370
H	-5.444268	-1.075907	-2.225415
H	-4.255875	-0.440413	-3.380124
H	-4.306096	0.200382	-1.729271
C	-1.519059	-1.619570	2.862179

H	-0.824092	-0.922267	2.380163
C	-0.769318	-2.910802	3.213798
H	-1.472560	-3.644510	3.624254
H	0.007625	-2.729971	3.963514
H	-0.304545	-3.352219	2.328256
C	-2.033354	-0.967430	4.151844
H	-2.690703	-0.114552	3.953263
H	-1.185284	-0.619026	4.753139
H	-2.590674	-1.681076	4.767774
C	0.314917	1.534028	0.397339
C	-3.355778	2.512477	-0.685419
C	-2.911488	2.333151	-1.959927
C	-4.333562	3.577650	-0.268879
H	-3.837399	4.356731	0.324827
H	-5.152329	3.186550	0.342656
H	-4.789999	4.068662	-1.127603
C	-3.468965	3.033970	-3.167949
H	-3.942979	2.317311	-3.852358
H	-2.700671	3.563181	-3.746251
H	-4.227570	3.766576	-2.897740
C	-3.224816	1.527402	1.641206
H	-2.523605	0.806198	2.086368
C	-3.173347	2.780549	2.535870
H	-2.255842	3.349620	2.344345
H	-3.193716	2.495558	3.596233
H	-4.024240	3.444556	2.363325
C	-4.604721	0.858466	1.722977
H	-5.408012	1.544629	1.439210
H	-4.806942	0.519171	2.746743
H	-4.643328	-0.009891	1.060152
C	-1.256772	1.258925	-3.448510
H	-1.971312	1.514004	-4.240362
C	-0.812642	-0.178043	-3.728329
H	-0.291032	-0.608485	-2.861583
H	-0.136050	-0.230995	-4.588505
H	-1.681496	-0.809501	-3.937538
C	-0.096179	2.257358	-3.542930
H	-0.469675	3.277348	-3.401108
H	0.430462	2.205929	-4.503869
H	0.620652	2.057267	-2.740176
C	0.411231	2.087779	1.721957
C	0.796748	2.842439	0.704126
Al	-1.363962	0.749656	-0.485238
C	1.265884	4.130705	0.145324

C	1.036817	5.307154	1.092986
H	0.762498	4.284272	-0.816425
H	2.334519	4.021117	-0.083366
H	1.383332	6.239673	0.640890
H	-0.027393	5.413164	1.323068
H	1.576343	5.160118	2.032921
C	0.117028	1.888876	3.161129
C	0.450134	3.104513	4.020636
H	0.670450	1.006060	3.502189
H	-0.942510	1.620882	3.248865
H	0.211810	2.911266	5.069614
H	1.515245	3.348663	3.950155
H	-0.123215	3.977935	3.695890

4

P	2.224240	0.177573	0.039362
Si	4.785959	0.142231	-0.475073
N	-1.235050	0.439321	-0.890774
N	3.643909	1.212703	0.300851
N	3.373150	-0.747736	-0.951894
N	-3.116862	-0.785019	1.382576
N	-1.872468	1.308113	2.259433
C	1.222175	1.022156	-1.197485
C	-0.124494	0.961658	-1.521393
C	-0.278593	1.779202	-2.813733
H	-1.193134	1.584845	-3.376148
C	-0.088701	3.270311	-2.394219
H	-0.348386	3.927918	-3.230422
H	-0.724481	3.542875	-1.548616
C	1.422539	3.349274	-2.050979
H	1.948263	4.035374	-2.724347
H	1.596041	3.678341	-1.025371
C	1.885354	1.886421	-2.270710
H	2.967124	1.760378	-2.337851
C	1.062962	1.514407	-3.511091
H	1.206034	0.474089	-3.813308
H	1.231412	2.176170	-4.369318
C	5.847492	0.876892	-1.837859
H	6.389216	0.089334	-2.374405
H	6.593907	1.562627	-1.420743
H	5.243162	1.429646	-2.562111
C	5.958823	-0.806962	0.663950
H	5.424991	-1.267524	1.501661

H	6.745754	-0.165413	1.076075
H	6.462896	-1.608538	0.109844
C	3.876141	2.106581	1.439379
C	2.818123	3.207592	1.450385
H	2.944882	3.858343	0.580561
H	2.889304	3.817123	2.358648
H	1.818325	2.772637	1.405799
C	3.860224	1.342045	2.772311
H	2.900722	0.833312	2.911225
H	4.012335	2.020479	3.619324
H	4.655101	0.587719	2.788319
C	5.250442	2.759732	1.251642
H	6.057757	2.019190	1.296269
H	5.433310	3.494052	2.043006
H	5.295732	3.270796	0.284492
C	3.210218	-2.120628	-1.409498
C	4.342875	-2.433428	-2.392768
H	4.331168	-1.717472	-3.220457
H	4.234943	-3.444715	-2.799052
H	5.320052	-2.377361	-1.897375
C	1.871717	-2.254506	-2.129343
H	1.050163	-1.968865	-1.462188
H	1.705917	-3.284028	-2.471173
H	1.837164	-1.582361	-2.990920
C	3.263283	-3.115233	-0.239307
H	4.228474	-3.057789	0.276177
H	3.113359	-4.147043	-0.581496
H	2.481121	-2.871811	0.487942
C	-2.452977	0.284023	-1.665060
C	-3.451776	1.282104	-1.645558
C	-4.632992	1.085093	-2.365726
H	-5.396302	1.858542	-2.343607
C	-4.847662	-0.068519	-3.104598
H	-5.769617	-0.202930	-3.661968
C	-3.869926	-1.052709	-3.114951
H	-4.033544	-1.960400	-3.689040
C	-2.680289	-0.903994	-2.398395
C	-3.298763	2.578198	-0.875007
H	-2.300154	2.582638	-0.433946
C	-3.429463	3.799044	-1.795476
H	-2.784113	3.715691	-2.674947
H	-3.157837	4.712614	-1.254324
H	-4.460759	3.917672	-2.146190
C	-4.316523	2.661580	0.268547

H	-5.336471	2.730262	-0.129023
H	-4.133636	3.556896	0.875314
H	-4.257652	1.787255	0.922832
C	-1.637532	-2.001370	-2.504698
H	-0.940143	-1.869138	-1.670377
C	-0.874243	-1.836755	-3.825243
H	-1.576733	-1.894638	-4.664685
H	-0.124071	-2.623417	-3.955201
H	-0.375335	-0.865428	-3.872592
C	-2.212621	-3.421354	-2.430330
H	-2.869103	-3.561621	-1.565438
H	-1.393671	-4.147652	-2.365923
H	-2.787602	-3.670328	-3.328378
C	-0.254624	-1.396361	1.440859
C	-3.740337	-0.127080	2.468816
C	-3.075255	0.969753	2.930414
C	-5.130214	-0.513846	2.896864
H	-5.235846	-1.589959	3.060618
H	-5.872543	-0.233690	2.137064
H	-5.415930	-0.028189	3.829815
C	-3.592481	1.905643	3.985398
H	-3.743765	2.916000	3.580159
H	-2.898739	2.001104	4.830969
H	-4.547092	1.573436	4.390287
C	-3.538803	-2.058768	0.830535
H	-2.797559	-2.260805	0.040581
C	-3.442869	-3.244889	1.805081
H	-2.479440	-3.239214	2.327289
H	-3.545006	-4.194874	1.264110
H	-4.226838	-3.219562	2.566176
C	-4.900655	-2.033175	0.121430
H	-5.730776	-2.084080	0.832018
H	-4.996021	-2.887252	-0.560709
H	-4.993339	-1.113058	-0.463424
C	-1.015535	2.374853	2.740994
H	-1.535428	2.959179	3.506596
C	-0.677799	3.340803	1.602607
H	-0.222171	2.802764	0.757850
H	0.020912	4.121620	1.923923
H	-1.593259	3.819360	1.239662
C	0.242429	1.787553	3.389613
H	-0.045727	1.151462	4.234562
H	0.937715	2.557589	3.745431
H	0.771157	1.160169	2.658291

C	0.041954	-2.759653	1.366396
C	0.563938	-2.031486	2.370548
Al	-1.563134	0.071605	0.932435
C	1.434600	-1.882297	3.559311
C	2.892886	-2.213316	3.211828
H	1.071636	-2.559737	4.340396
H	1.347567	-0.858543	3.931968
H	3.528691	-2.037176	4.082977
H	2.997767	-3.258644	2.906945
H	3.241996	-1.577124	2.392844
C	-0.121132	-4.032022	0.629558
C	0.478403	-5.229126	1.361681
H	0.348526	-3.889115	-0.353320
H	-1.191491	-4.165990	0.429878
H	0.342168	-6.144184	0.780843
H	1.551033	-5.083602	1.523987
H	-0.001061	-5.368249	2.334920

TS(4-->3)

P	2.311247	-0.030041	0.124737
Si	4.833463	-0.140297	-0.513152
N	-1.271396	-0.869250	-0.393481
N	3.445576	0.861389	-0.877237
N	3.669074	-1.113046	0.348696
N	-3.236474	0.863691	1.312775
N	-2.672230	2.174498	-0.855390
C	1.201364	-0.889985	-1.010987
C	-0.137429	-1.263456	-1.058901
C	-0.262208	-2.232581	-2.247789
H	-1.147788	-2.868117	-2.217351
C	-0.150053	-1.338604	-3.519402
H	-0.382012	-1.932148	-4.409686
H	-0.847167	-0.498714	-3.490590
C	1.339963	-0.898789	-3.502185
H	1.872475	-1.266729	-4.386179
H	1.462668	0.186135	-3.461876
C	1.866747	-1.578405	-2.212462
H	2.952335	-1.644409	-2.145246
C	1.107534	-2.911153	-2.264186
H	1.288570	-3.550438	-1.398116
H	1.289180	-3.479571	-3.183818
C	5.714146	-0.875018	-2.000719
H	6.478452	-1.598730	-1.697940

H	6.223449	-0.075755	-2.552296
H	5.025821	-1.369128	-2.690988
C	6.171019	0.608846	0.580354
H	5.750383	1.047614	1.490632
H	6.741176	1.384485	0.055791
H	6.888278	-0.165461	0.879674
C	3.405346	2.292530	-1.184491
C	2.018854	2.670343	-1.701568
H	1.797975	2.135125	-2.628952
H	1.950146	3.746789	-1.896736
H	1.241025	2.406904	-0.977759
C	3.763093	3.125067	0.056895
H	3.138967	2.822115	0.904350
H	3.620593	4.197997	-0.119208
H	4.808380	2.964494	0.339557
C	4.433511	2.560535	-2.288501
H	5.449769	2.327859	-1.945905
H	4.417923	3.615864	-2.579890
H	4.213404	1.946607	-3.167420
C	3.851260	-2.301476	1.184690
C	4.868141	-3.209359	0.480987
H	4.528179	-3.447044	-0.532348
H	5.003354	-4.142282	1.037589
H	5.848794	-2.721039	0.414167
C	2.540598	-3.060609	1.347959
H	1.779549	-2.441622	1.837176
H	2.699021	-3.949345	1.968069
H	2.145352	-3.371622	0.379523
C	4.387898	-1.931077	2.574062
H	5.290601	-1.316324	2.493080
H	4.633529	-2.831367	3.148314
H	3.637434	-1.367213	3.134384
C	-2.350689	-1.833143	-0.297009
C	-3.480064	-1.763149	-1.141974
C	-4.546073	-2.640860	-0.930009
H	-5.415187	-2.576698	-1.579635
C	-4.515048	-3.589205	0.082069
H	-5.355948	-4.258380	0.236359
C	-3.387002	-3.680932	0.884064
H	-3.344424	-4.439800	1.661151
C	-2.298462	-2.822739	0.710328
C	-3.574482	-0.801558	-2.311504
H	-2.685656	-0.168143	-2.294615
C	-3.599809	-1.557977	-3.647094

H	-2.748012	-2.236486	-3.750787
H	-3.577218	-0.849939	-4.483682
H	-4.515032	-2.153746	-3.739003
C	-4.797827	0.114565	-2.200579
H	-5.723119	-0.448235	-2.373560
H	-4.741746	0.905727	-2.957915
H	-4.853157	0.587886	-1.216579
C	-1.055878	-3.072345	1.549827
H	-0.351459	-2.254775	1.362360
C	-0.419480	-4.392180	1.088894
H	-1.129877	-5.216148	1.218190
H	0.476188	-4.628305	1.670934
H	-0.150693	-4.351640	0.028473
C	-1.322581	-3.139485	3.058592
H	-1.798857	-2.230755	3.436497
H	-0.376825	-3.277965	3.595621
H	-1.967861	-3.986946	3.313454
C	-0.197917	1.567902	1.059048
C	-4.160222	1.875480	0.964466
C	-3.856733	2.567842	-0.169924
C	-5.453619	2.011829	1.720672
H	-5.294352	2.034056	2.803275
H	-6.131463	1.172439	1.516353
H	-5.978474	2.931341	1.460440
C	-4.764378	3.561226	-0.839371
H	-5.125902	3.177384	-1.804192
H	-4.262036	4.514604	-1.048368
H	-5.640676	3.786349	-0.232405
C	-3.254381	0.077505	2.530671
H	-2.418361	-0.625515	2.395409
C	-2.922669	0.879303	3.798253
H	-1.998390	1.448923	3.647628
H	-2.788262	0.211598	4.658414
H	-3.713756	1.592142	4.049655
C	-4.496061	-0.804821	2.723287
H	-5.345492	-0.245125	3.125313
H	-4.275192	-1.619704	3.423789
H	-4.784433	-1.246442	1.764155
C	-2.148225	3.017906	-1.909359
H	-2.970948	3.418878	-2.518213
C	-1.273695	2.187100	-2.848498
H	-0.538922	1.595274	-2.281259
H	-0.716555	2.821783	-3.547100
H	-1.887514	1.491104	-3.428760

C	-1.362985	4.212337	-1.350888
H	-1.972923	4.762762	-0.626522
H	-1.044204	4.902803	-2.141298
H	-0.470634	3.848619	-0.829989
C	0.938882	1.272461	1.853122
C	0.602577	2.572157	1.496672
Al	-1.842066	0.869264	0.144116
C	0.811724	4.041865	1.557523
C	1.640548	4.509723	2.751788
H	-0.181427	4.504640	1.559549
H	1.283012	4.354688	0.616473
H	1.692094	5.601172	2.773291
H	1.194476	4.173348	3.692666
H	2.662801	4.123667	2.700116
C	1.384088	0.534936	3.074272
C	2.739888	1.022340	3.577540
H	1.379185	-0.543060	2.887600
H	0.609747	0.732252	3.830375
H	3.056667	0.464507	4.462901
H	3.503696	0.896724	2.801574
H	2.689864	2.082226	3.842069

3

Al	-1.562674	0.942510	0.232871
P	2.353270	0.023532	-0.092992
Si	4.643238	-0.630946	0.859508
N	-1.165183	-0.763636	-0.646395
N	3.979093	0.060440	-0.619320
N	2.961994	-0.683338	1.338134
N	-2.199501	0.662941	1.950897
N	-3.133442	1.709309	-0.351764
C	1.330145	-0.990333	-1.085063
C	-0.048819	-1.311511	-1.140574
C	-0.133298	-2.567339	-2.019578
H	-1.070012	-3.114491	-1.914416
C	0.175284	-2.099680	-3.470712
H	-0.067692	-2.899033	-4.177497
H	-0.410636	-1.221195	-3.748851
C	1.694213	-1.806802	-3.429023
H	1.913343	-0.788398	-3.743702
H	2.252775	-2.491402	-4.077407
C	2.039821	-2.062888	-1.936479
H	3.109502	-2.163841	-1.737954

C	1.166412	-3.298075	-1.668347
H	1.373095	-4.134317	-2.346353
H	1.206861	-3.646981	-0.634543
C	5.493176	-2.284918	0.643248
H	5.648396	-2.781732	1.607721
H	6.477019	-2.162165	0.177163
H	4.892594	-2.946448	0.011226
C	5.713636	0.508471	1.892297
H	5.196727	1.454320	2.081435
H	6.672749	0.727609	1.410659
H	5.934923	0.044914	2.860223
C	4.645596	0.857789	-1.661875
C	6.047954	0.269445	-1.853961
H	6.653948	0.375193	-0.945801
H	6.571018	0.793847	-2.659663
H	5.983880	-0.792541	-2.112829
C	3.887428	0.735903	-2.981238
H	3.964466	-0.284430	-3.366198
H	4.302542	1.422589	-3.726491
H	2.825678	0.966505	-2.849349
C	4.769189	2.327813	-1.241737
H	3.783169	2.773392	-1.085765
H	5.292989	2.906843	-2.010122
H	5.332690	2.411258	-0.305681
C	2.281198	-1.376525	2.440743
C	2.041723	-2.845642	2.080645
H	1.399003	-2.911948	1.200885
H	1.554133	-3.376037	2.906820
H	2.989369	-3.348084	1.855208
C	0.959890	-0.683901	2.761418
H	1.136363	0.327745	3.136316
H	0.419272	-1.240091	3.532586
H	0.297626	-0.619335	1.888508
C	3.196478	-1.294123	3.667093
H	4.146604	-1.814614	3.488094
H	2.718822	-1.770160	4.529003
H	3.411112	-0.250144	3.919094
C	-2.400199	-1.528513	-0.644757
C	-3.402259	-1.295224	-1.610523
C	-4.666275	-1.855507	-1.411625
H	-5.447487	-1.668244	-2.143302
C	-4.941709	-2.652868	-0.309755
H	-5.936977	-3.061367	-0.163572
C	-3.917977	-2.964982	0.572993

H	-4.109356	-3.644732	1.399083
C	-2.639136	-2.427976	0.416463
C	-3.126141	-0.593496	-2.928661
H	-2.160905	-0.080457	-2.841233
C	-4.187015	0.439337	-3.313743
H	-5.145435	-0.041891	-3.538519
H	-3.878321	0.980851	-4.215091
H	-4.337876	1.152491	-2.505695
C	-3.044675	-1.652473	-4.042722
H	-4.038523	-2.080371	-4.216333
H	-2.375265	-2.476295	-3.784244
H	-2.700754	-1.206509	-4.983041
C	-1.530390	-2.924279	1.327133
H	-0.634175	-2.337667	1.114616
C	-1.219607	-4.396029	1.016624
H	-2.076832	-5.031529	1.265815
H	-0.362852	-4.741230	1.607425
H	-0.990487	-4.548627	-0.043042
C	-1.856517	-2.746091	2.809241
H	-2.021568	-1.686194	3.014409
H	-1.029672	-3.114166	3.429507
H	-2.753468	-3.307501	3.094149
C	0.154675	1.824367	-0.116959
C	1.662788	1.661583	0.233425
C	1.024417	2.394321	-0.900359
C	1.300890	3.284989	-2.063321
H	0.450428	3.233588	-2.750132
H	2.177898	2.929807	-2.612811
C	1.532525	4.738803	-1.633374
H	0.656497	5.126058	-1.104693
H	1.717500	5.370976	-2.506193
H	2.396095	4.819189	-0.964654
C	2.305001	2.400252	1.417082
H	2.451312	1.705123	2.251009
H	3.311591	2.737479	1.130433
C	1.485144	3.596110	1.894323
H	1.376499	4.351349	1.111077
H	1.965956	4.066549	2.756669
H	0.477219	3.287490	2.188964
C	-3.623078	0.714432	1.761152
C	-4.086162	1.262148	0.606755
C	-4.504710	0.063375	2.799818
H	-5.445570	-0.296295	2.376827
H	-4.754428	0.741497	3.627878

H	-3.992010	-0.801864	3.231622
C	-5.536939	1.328041	0.209801
H	-5.699397	0.810859	-0.744541
H	-5.867504	2.365947	0.076827
H	-6.190678	0.877704	0.956970
C	-1.665194	1.422758	3.090770
H	-0.585063	1.506240	2.906686
C	-1.815207	0.740600	4.458421
H	-2.857319	0.727489	4.790408
H	-1.235483	1.284492	5.213717
H	-1.455094	-0.290921	4.431336
C	-2.215324	2.851700	3.169233
H	-2.023266	3.388740	2.235048
H	-1.756459	3.408497	3.994614
H	-3.300122	2.838183	3.323126
C	-3.421602	2.953033	-1.046801
H	-4.394463	2.880415	-1.561167
C	-2.358216	3.210496	-2.108417
H	-1.399353	3.406599	-1.616589
H	-2.611972	4.083165	-2.719404
H	-2.237838	2.342299	-2.765986
C	-3.504933	4.156957	-0.100064
H	-4.164317	3.941112	0.747245
H	-3.877823	5.048442	-0.618044
H	-2.508737	4.382755	0.300038

TS(INT5-->5)

P	2.002202	-0.249575	-0.119800
Si	4.444696	-0.508749	0.646330
N	-1.281974	-0.982833	-0.430398
N	3.561242	-0.020246	-0.794956
N	2.842227	-0.645210	1.325750
N	-2.356498	1.395027	1.101086
N	-1.786761	2.272213	-1.266261
C	1.115214	-1.575374	-0.831447
C	-0.263082	-1.772492	-0.835979
C	-0.480493	-3.117314	-1.533084
H	-1.459753	-3.567309	-1.373652
C	-0.150374	-2.843373	-3.031869
H	-0.489853	-3.678534	-3.651970
H	-0.648322	-1.936133	-3.387875
C	1.396899	-2.714329	-3.036069
H	1.862600	-3.547487	-3.574770

H	1.732672	-1.788207	-3.503717
C	1.736863	-2.788347	-1.519395
H	2.794545	-2.954436	-1.296926
C	0.763179	-3.900582	-1.091365
H	0.790138	-4.104436	-0.018616
H	0.896784	-4.835303	-1.648324
C	5.421466	-2.104952	0.507196
H	5.688993	-2.476707	1.503634
H	6.357588	-1.954605	-0.042488
H	4.844505	-2.882696	-0.002106
C	5.551575	0.774769	1.449114
H	5.019481	1.713374	1.626189
H	6.433486	0.990282	0.836890
H	5.909827	0.404828	2.416650
C	4.007470	0.316158	-2.156163
C	2.850071	0.870867	-2.988375
H	2.024807	0.155869	-3.039881
H	3.193303	1.077052	-4.007296
H	2.451971	1.794792	-2.560376
C	5.117931	1.369328	-2.055487
H	4.768385	2.255260	-1.518344
H	5.451053	1.670832	-3.053998
H	5.988737	0.965550	-1.524414
C	4.583839	-0.931246	-2.840879
H	5.422511	-1.333405	-2.261642
H	4.952247	-0.685740	-3.842968
H	3.826963	-1.713183	-2.932158
C	2.302937	-1.198547	2.570716
C	2.168256	-2.722541	2.463084
H	1.507667	-2.978091	1.629583
H	1.753729	-3.147898	3.384535
H	3.145904	-3.182130	2.277728
C	0.941203	-0.568487	2.871753
H	1.033828	0.521342	2.903972
H	0.559173	-0.926682	3.834277
H	0.201395	-0.817062	2.100251
C	3.278787	-0.844674	3.696620
H	4.265231	-1.290377	3.513252
H	2.915426	-1.229676	4.654745
H	3.395711	0.241353	3.774342
C	-2.560301	-1.623005	-0.235356
C	-3.646558	-1.303177	-1.075041
C	-4.901894	-1.863223	-0.822436
H	-5.732395	-1.605356	-1.474754

C	-5.101032	-2.745027	0.228444
H	-6.082955	-3.167607	0.417411
C	-4.018067	-3.099079	1.021723
H	-4.160172	-3.814908	1.827689
C	-2.745390	-2.565077	0.809199
C	-3.485908	-0.427808	-2.300112
H	-2.468108	-0.039046	-2.294648
C	-3.667458	-1.259085	-3.577253
H	-2.992176	-2.121008	-3.592315
H	-3.468639	-0.648252	-4.465539
H	-4.693038	-1.638003	-3.654978
C	-4.439957	0.769557	-2.289834
H	-5.477564	0.449457	-2.443755
H	-4.181424	1.462081	-3.100618
H	-4.375977	1.314640	-1.343250
C	-1.614416	-3.094215	1.685434
H	-0.683417	-2.605027	1.385882
C	-1.437704	-4.609493	1.489144
H	-2.286808	-5.154088	1.916402
H	-0.531098	-4.955376	1.999683
H	-1.365158	-4.884195	0.433919
C	-1.827244	-2.825834	3.182189
H	-1.889131	-1.760014	3.412874
H	-0.994253	-3.247207	3.757364
H	-2.748499	-3.301659	3.536238
C	0.906857	1.097008	-0.098331
C	-3.033722	2.550347	0.717768
C	-2.704555	3.023975	-0.534825
C	-4.053828	3.217123	1.608584
H	-4.075751	4.298381	1.455117
H	-3.825155	3.056802	2.664458
H	-5.072331	2.841832	1.443281
C	-3.366556	4.214900	-1.171121
H	-3.974383	3.904680	-2.032431
H	-2.644803	4.951913	-1.543624
H	-4.034016	4.725460	-0.477600
C	-2.718569	0.566799	2.241346
H	-2.178115	-0.369174	2.059151
C	-2.216489	1.059962	3.606349
H	-1.130785	1.181851	3.581589
H	-2.461170	0.325302	4.383563
H	-2.660813	2.014096	3.907516
C	-4.202897	0.183653	2.305361
H	-4.817506	0.978899	2.736943

H	-4.326488	-0.708329	2.930610
H	-4.577343	-0.049325	1.303977
C	-1.282519	2.795285	-2.525257
H	-2.100323	3.291548	-3.067095
C	-0.778203	1.659075	-3.418335
H	-0.108337	1.001749	-2.847632
H	-0.211688	2.056583	-4.267959
H	-1.604038	1.059674	-3.812371
C	-0.163042	3.828394	-2.323415
H	-0.434223	4.554035	-1.549425
H	0.053721	4.365754	-3.254008
H	0.747941	3.316061	-1.998123
C	0.295071	2.696394	1.139707
C	1.322972	2.425951	0.367580
Al	-1.055519	0.951378	-0.157486
C	2.571561	3.202464	0.046811
C	2.521184	4.655231	0.510255
H	2.732534	3.165142	-1.036776
H	3.427402	2.677433	0.491225
H	3.437025	5.185596	0.235815
H	1.675920	5.173519	0.045838
H	2.405723	4.724406	1.596240
C	-0.168375	3.499804	2.288867
C	0.628900	3.348098	3.588804
H	-1.242110	3.357784	2.450611
H	-0.061030	4.536493	1.926732
H	0.271896	4.059707	4.339833
H	0.528091	2.344611	4.008852
H	1.693944	3.531031	3.414995

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Al	-1.046545	0.735848	0.357575
P	1.939775	-0.121908	0.099172
Si	4.471361	-0.294597	-0.454210
N	-1.334726	-1.131237	0.297190
N	2.940714	-0.470684	-1.270114
N	3.465779	0.083331	0.923566
N	-1.682965	1.968385	-1.121972
N	-2.008795	1.788990	1.547823
C	1.099598	-1.558839	0.735318
C	-0.239465	-1.882371	0.654300
C	-0.393222	-3.275508	1.264090
H	-1.310301	-3.799668	0.990564

C	-0.215551	-3.061143	2.795652
H	-0.860849	-2.256860	3.163656
H	-0.475262	-3.974992	3.339348
C	1.295354	-2.727187	2.924691
H	1.823228	-3.490422	3.507811
H	1.460326	-1.762810	3.409276
C	1.772954	-2.733227	1.439249
H	2.856683	-2.787508	1.311177
C	0.952309	-3.917298	0.899910
H	1.085948	-4.071002	-0.173705
H	1.134560	-4.855754	1.436460
C	5.520039	-1.848894	-0.320591
H	4.933961	-2.688620	0.065532
H	6.376617	-1.693600	0.345574
H	5.921820	-2.135463	-1.299676
C	5.561376	1.099776	-1.083830
H	5.882863	0.910954	-2.113876
H	6.464645	1.212696	-0.475056
H	5.017668	2.049908	-1.063685
C	2.575261	-0.967898	-2.598350
C	3.721706	-0.633453	-3.558173
H	3.877851	0.449542	-3.606003
H	3.494449	-0.998352	-4.565058
H	4.657753	-1.108425	-3.237665
C	2.375524	-2.488662	-2.550643
H	3.299146	-2.984067	-2.229460
H	2.090175	-2.885046	-3.532932
H	1.591066	-2.735229	-1.829182
C	1.300168	-0.291396	-3.111002
H	0.451318	-0.520931	-2.461493
H	1.072358	-0.642577	-4.123878
H	1.416163	0.797214	-3.130601
C	3.839148	0.410944	2.306479
C	2.654511	1.005782	3.066324
H	2.327296	1.947045	2.617748
H	2.935981	1.193634	4.108007
H	1.805123	0.317982	3.058593
C	4.990174	1.427916	2.286802
H	5.886747	0.990324	1.830395
H	5.253264	1.722453	3.308303
H	4.720864	2.324814	1.722479
C	4.342856	-0.843865	3.036469
H	3.556010	-1.594319	3.123941
H	4.690972	-0.589704	4.044116

H	5.181139	-1.291377	2.490790
C	-2.533548	-1.825500	-0.076083
C	-2.579806	-2.570575	-1.278868
C	-3.791393	-3.137894	-1.679516
H	-3.826456	-3.707817	-2.604736
C	-4.948848	-2.987772	-0.927300
H	-5.884220	-3.423540	-1.264337
C	-4.885096	-2.299013	0.275207
H	-5.776043	-2.209444	0.891799
C	-3.691220	-1.731024	0.725494
C	-1.353522	-2.828770	-2.140454
H	-0.514951	-2.270344	-1.716609
C	-0.992447	-4.321845	-2.125400
H	-0.906740	-4.708162	-1.106462
H	-0.040743	-4.492224	-2.641752
H	-1.762951	-4.907676	-2.639557
C	-1.536409	-2.372050	-3.592478
H	-2.348228	-2.921238	-4.081716
H	-0.618843	-2.558235	-4.161816
H	-1.763833	-1.304349	-3.660775
C	-3.670607	-1.076358	2.091169
H	-2.679101	-0.647326	2.229513
C	-3.894960	-2.122050	3.191038
H	-4.899111	-2.555792	3.121818
H	-3.794761	-1.665280	4.182517
H	-3.171377	-2.940061	3.113606
C	-4.688394	0.061710	2.208104
H	-4.581984	0.773014	1.383504
H	-4.537484	0.606855	3.147803
H	-5.715577	-0.321663	2.205081
C	0.768042	1.052520	-0.092308
C	-2.719687	2.807006	-0.490036
C	-2.774823	2.727324	0.863583
C	-3.615341	3.693080	-1.324014
H	-4.664499	3.594168	-1.025646
H	-3.569805	3.423973	-2.379422
H	-3.350133	4.756869	-1.256484
C	-3.692703	3.618851	1.661263
H	-3.121126	4.334178	2.263593
H	-4.296483	3.019803	2.351234
H	-4.362741	4.191501	1.020181
C	-2.136798	1.075841	-2.264623
H	-1.485189	0.194933	-2.184561
C	-1.920989	1.630003	-3.672481

H	-2.584327	2.467172	-3.907981
H	-2.137548	0.832104	-4.390881
H	-0.885136	1.944759	-3.821271
C	-3.576473	0.607809	-2.061061
H	-3.776227	0.328121	-1.022451
H	-3.757175	-0.278839	-2.676910
H	-4.297059	1.376924	-2.351426
C	-1.519189	2.136887	2.880806
H	-2.343431	2.536656	3.489011
C	-1.003309	0.884981	3.591907
H	-1.824304	0.222777	3.882339
H	-0.444881	1.154248	4.494270
H	-0.320561	0.316610	2.943127
C	-0.421009	3.203624	2.784352
H	0.405618	2.811965	2.180869
H	-0.042424	3.490693	3.772045
H	-0.797148	4.101710	2.281287
C	0.748231	2.242321	-0.934797
C	-0.432581	2.726060	-1.417509
C	2.049312	2.955462	-1.247674
H	1.911057	3.748049	-1.987910
H	2.732748	2.218424	-1.693505
C	2.701526	3.532779	0.010589
H	2.034713	4.245651	0.507535
H	3.639906	4.046226	-0.227046
H	2.916186	2.726133	0.714480
C	-0.591803	4.043599	-2.144923
H	-1.549946	4.063673	-2.666371
H	0.163092	4.136290	-2.934871
C	-0.501438	5.261548	-1.215995
H	-1.223056	5.170237	-0.397450
H	-0.697685	6.193758	-1.756787
H	0.494994	5.330739	-0.769091

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C	-2.950020	-1.466522	-0.937673
C	-1.643889	-1.114229	-0.997200
C	-2.373233	-1.258940	-2.199553
N	-4.073086	-1.798720	-0.268769
N	-0.452763	-0.823604	-0.459581
C	-5.172368	-2.309669	-1.109272
C	-6.484420	-1.538415	-0.943139
C	-5.378025	-3.820429	-0.982761

H	-4.812812	-2.112864	-2.123968
H	-6.295202	-0.461670	-0.931660
H	-7.141194	-1.761557	-1.790078
H	-7.022160	-1.810435	-0.031545
H	-4.437295	-4.354049	-1.147110
H	-5.772094	-4.100710	-0.000333
H	-6.099420	-4.157387	-1.734008
C	-3.937296	-2.012579	1.179238
C	-3.199485	-3.314259	1.511045
C	-5.253234	-1.905728	1.942774
H	-3.310329	-1.179025	1.519771
H	-2.276878	-3.390516	0.925214
H	-2.935411	-3.343283	2.573751
H	-3.817363	-4.189465	1.290360
H	-5.758849	-0.960391	1.731718
H	-5.933553	-2.728863	1.706806
H	-5.042360	-1.952033	3.015378
C	-0.215995	-0.913657	0.981682
C	0.210585	0.434186	1.564831
C	0.779247	-2.024587	1.321148
H	-1.184169	-1.182890	1.415483
H	-0.529711	1.203999	1.330304
H	0.312170	0.364188	2.652232
H	1.177759	0.753182	1.161790
H	0.437186	-2.982913	0.919322
H	1.769097	-1.811164	0.902962
H	0.889748	-2.119721	2.405866
C	0.655745	-0.497908	-1.374480
C	0.338959	0.764983	-2.173806
C	0.974912	-1.681255	-2.287845
H	1.525236	-0.300874	-0.737477
H	0.141927	1.606834	-1.502833
H	1.180392	1.025082	-2.823517
H	-0.545208	0.596698	-2.795371
H	1.224718	-2.569329	-1.698713
H	0.107427	-1.908014	-2.914339
H	1.824015	-1.443412	-2.936212

7 Triplet

C	-2.311174	-3.148057	-0.295852
C	-1.098735	-2.478703	-0.920634
C	-1.807576	-3.322853	-1.662080
N	-3.421192	-2.460096	0.188516

N	-0.214332	-1.516673	-0.626331
C	-4.377244	-1.938188	-0.806648
C	-4.685491	-0.446995	-0.638285
C	-5.658462	-2.765520	-0.937522
H	-3.838249	-2.038854	-1.754419
H	-3.760680	0.123201	-0.510092
H	-5.191678	-0.077094	-1.536550
H	-5.338415	-0.245407	0.214339
H	-5.421682	-3.821901	-1.091764
H	-6.299145	-2.673905	-0.054770
H	-6.233914	-2.412120	-1.799582
C	-3.790945	-2.827108	1.564642
C	-4.404985	-4.227804	1.682868
C	-4.649477	-1.778034	2.264975
H	-2.829924	-2.860788	2.093463
H	-3.796838	-4.945111	1.124369
H	-4.430034	-4.537105	2.733270
H	-5.428262	-4.260071	1.299513
H	-4.195014	-0.784920	2.203157
H	-5.658908	-1.726339	1.846074
H	-4.748590	-2.046527	3.321198
C	-0.038631	-1.142044	0.784466
C	-0.888487	0.070509	1.163441
C	1.436626	-0.944671	1.126482
H	-0.405746	-2.008211	1.345335
H	-1.941176	-0.130108	0.938799
H	-0.792458	0.288039	2.232087
H	-0.570476	0.962023	0.610353
H	2.022924	-1.813689	0.816538
H	1.851301	-0.053927	0.643215
H	1.551336	-0.812360	2.206489
C	0.209806	-0.614776	-1.712952
C	-0.983196	0.100912	-2.348069
C	1.010119	-1.399469	-2.749386
H	0.863164	0.130967	-1.247686
H	-1.538356	0.679971	-1.604100
H	-0.646711	0.780319	-3.137023
H	-1.663722	-0.633404	-2.792493
H	1.882811	-1.868350	-2.286978
H	0.386181	-2.186682	-3.185133
H	1.346936	-0.739991	-3.554805

INT6

Al	0.858989	1.082527	0.894479
P	-0.503345	-1.843655	-0.130756
Si	-1.560555	-4.214096	-0.365548
N	1.972008	0.491507	-0.527430
N	-1.816232	-2.623725	-1.023388
C	0.656428	-1.443375	-1.435513
C	1.634489	-0.472140	-1.452970
C	2.381758	-0.639659	-2.779750
H	2.965939	0.229665	-3.087912
C	3.197927	-1.963530	-2.711859
H	3.810602	-2.055316	-3.614538
H	3.867796	-1.993386	-1.855349
C	2.096532	-3.059547	-2.663956
H	2.182296	-3.744233	-3.515715
H	2.119319	-3.653545	-1.746123
C	0.794077	-2.220069	-2.743270
H	-0.095091	-2.793770	-3.016504
C	1.228759	-1.093413	-3.695362
H	1.582814	-1.447540	-4.671707
H	0.457994	-0.330264	-3.832826
C	-1.232972	-5.589497	-1.599932
H	-2.133684	-5.852307	-2.166202
H	-0.887493	-6.495501	-1.088440
H	-0.455525	-5.281206	-2.306148
C	-2.910574	-4.795033	0.817779
H	-3.157695	-4.003395	1.533065
H	-2.606199	-5.681562	1.385903
H	-3.826043	-5.061143	0.275654
N	-0.150229	-3.504966	0.364983
C	0.598623	-3.870060	1.566453
C	1.970127	-3.201351	1.525805
H	2.507441	-3.482994	0.613650
H	2.570353	-3.490137	2.396777
H	1.858996	-2.109065	1.542367
C	-0.125383	-3.428291	2.846912
H	-0.221962	-2.336797	2.860595
H	0.434051	-3.730287	3.740143
H	-1.127446	-3.869038	2.899317
C	0.772406	-5.391548	1.559284
H	-0.198790	-5.899256	1.616519
H	1.367410	-5.717411	2.418720
H	1.276783	-5.709036	0.640503
C	-2.949573	-1.980643	-1.665981
C	-2.460106	-0.876573	-2.604980

H	-1.871688	-0.138444	-2.052089
H	-3.310993	-0.366419	-3.071951
H	-1.821068	-1.292193	-3.390884
C	-3.896625	-1.372535	-0.620722
H	-4.294561	-2.156337	0.035170
H	-4.741207	-0.853786	-1.094538
H	-3.348451	-0.658634	0.004465
C	-3.698497	-3.038082	-2.482782
H	-3.030737	-3.482640	-3.228186
H	-4.555413	-2.593905	-3.000511
H	-4.077988	-3.837731	-1.834782
C	3.303355	1.050705	-0.644461
C	4.433910	0.286860	-0.257090
C	5.715656	0.810797	-0.424978
H	6.572568	0.213180	-0.129545
C	5.917231	2.084697	-0.935594
H	6.921012	2.480532	-1.055819
C	4.813335	2.845885	-1.276158
H	4.959330	3.850047	-1.665247
C	3.510780	2.351788	-1.147228
C	4.298921	-1.036977	0.467494
H	3.353596	-1.493142	0.168179
C	5.429288	-2.036444	0.191323
H	5.673115	-2.120887	-0.871966
H	5.138187	-3.026878	0.557701
H	6.346019	-1.755955	0.721500
C	4.241099	-0.746987	1.971477
H	4.139412	-1.672744	2.548367
H	3.400834	-0.090212	2.210199
H	5.165464	-0.247388	2.286430
C	2.386710	3.269838	-1.587182
H	1.445314	2.728981	-1.455646
C	2.533760	3.625005	-3.072859
H	1.714388	4.269998	-3.409516
H	2.541977	2.723841	-3.695393
H	3.467959	4.165329	-3.257279
C	2.352826	4.532261	-0.716320
H	2.146688	4.269133	0.325793
H	1.585152	5.233209	-1.060567
H	3.314077	5.055609	-0.752029
C	-1.078175	1.525024	0.332167
C	-1.578319	3.103412	-2.539995
H	-2.167747	3.526257	-3.357402
C	-3.998200	2.642798	-1.853064

H	-4.471586	1.823378	-1.302041
C	-4.682498	1.825674	1.611701
H	-4.765415	2.134225	0.569888
C	-2.873364	0.893300	3.115615
H	-3.807205	0.794590	3.677114
C	1.098736	0.950287	2.795789
C	1.546030	2.145233	2.323926
C	1.005357	0.375596	4.195155
H	0.990068	1.169367	4.952171
H	0.049802	-0.155136	4.294103
C	2.114666	-0.617759	4.549123
H	2.135797	-1.445515	3.833161
H	1.955760	-1.035270	5.549261
H	3.098789	-0.138118	4.531390
C	2.192402	3.346666	2.962356
H	3.167764	3.487284	2.473841
H	1.613432	4.241063	2.689242
C	2.390063	3.321988	4.480127
H	1.429280	3.311580	5.004603
H	2.944958	4.204326	4.817039
H	2.950253	2.432812	4.787332
C	-2.121449	1.970288	-0.475258
C	-2.394395	1.574001	0.818855
N	-2.553320	2.452291	-1.641400
N	-3.284979	1.391624	1.783266
C	-1.988579	1.911066	3.830886
H	-1.056230	2.071865	3.281241
H	-2.509272	2.867520	3.940385
H	-1.728263	1.542698	4.827876
C	-2.240667	-0.486047	2.988058
H	-2.048229	-0.901810	3.981873
H	-2.906172	-1.169056	2.447629
H	-1.290786	-0.426394	2.446419
C	-5.668940	0.680339	1.840424
H	-6.676954	1.010496	1.571730
H	-5.410811	-0.186545	1.227183
H	-5.696251	0.368482	2.888764
C	-5.000047	3.035572	2.490411
H	-4.955408	2.776635	3.553427
H	-4.292500	3.849532	2.305630
H	-6.010998	3.395921	2.276509
C	-0.887044	4.254969	-1.815301
H	-0.187268	4.760967	-2.485553
H	-1.622814	4.987337	-1.468107

H	-0.326515	3.896567	-0.946882
C	-0.622512	2.071804	-3.129475
H	-1.175809	1.356438	-3.745510
H	0.129673	2.560941	-3.754437
H	-0.102872	1.509469	-2.344471
C	-4.397812	2.473724	-3.319397
H	-3.905497	1.606662	-3.766761
H	-5.479650	2.324490	-3.377296
H	-4.161303	3.358685	-3.917083
C	-4.474914	3.987940	-1.303828
H	-4.048168	4.808264	-1.891335
H	-5.565690	4.065701	-1.359770
H	-4.168284	4.123712	-0.261313

TS(INT6-->INT7)

Al	-0.185502	1.311212	0.699952
P	1.276363	-1.767554	0.152794
Si	2.088034	-4.227230	-0.125715
N	1.302341	1.628559	-0.366140
N	0.842838	-3.203684	-0.772367
C	1.949329	-0.678044	-1.112929
C	1.934701	0.692573	-1.168237
C	2.807346	1.094748	-2.355419
H	2.670191	2.121023	-2.700810
C	4.280327	0.733265	-1.998766
H	4.949724	1.117421	-2.774828
H	4.589926	1.174225	-1.049178
C	4.270490	-0.822348	-1.978016
H	4.940186	-1.230214	-2.743824
H	4.559578	-1.247110	-1.013348
C	2.787870	-1.145571	-2.300319
H	2.598594	-2.179331	-2.601259
C	2.467848	-0.047577	-3.330652
H	3.120804	-0.063267	-4.212032
H	1.418227	-0.045171	-3.641182
C	3.308395	-4.978594	-1.338384
H	2.836424	-5.740750	-1.968573
H	4.133339	-5.460339	-0.800175
H	3.733605	-4.205733	-1.985685
C	1.459314	-5.617600	0.982024
H	0.680026	-5.251529	1.658245
H	2.259324	-6.058578	1.588066
H	1.032034	-6.427797	0.379040

N	2.635432	-2.772784	0.672636
C	3.324986	-2.620136	1.955098
C	3.778057	-1.170668	2.108974
H	4.408817	-0.872540	1.264760
H	4.338739	-1.030077	3.040390
H	2.904073	-0.509659	2.137836
C	2.417591	-2.984365	3.140835
H	1.508252	-2.372996	3.118040
H	2.926983	-2.809173	4.095238
H	2.125034	-4.038108	3.099051
C	4.549639	-3.539322	1.934557
H	4.248904	-4.590585	1.841182
H	5.125191	-3.440891	2.861080
H	5.195572	-3.288687	1.086898
C	-0.387160	-3.447568	-1.511653
C	-0.656822	-2.275741	-2.451792
H	-0.776957	-1.351926	-1.878696
H	-1.578695	-2.437418	-3.021476
H	0.178235	-2.139954	-3.148271
C	-1.577232	-3.612615	-0.555680
H	-1.415170	-4.465790	0.114047
H	-2.509823	-3.776552	-1.111898
H	-1.694471	-2.711505	0.056449
C	-0.199809	-4.726612	-2.332340
H	0.644713	-4.615697	-3.021005
H	-1.099806	-4.945467	-2.916379
H	-0.008414	-5.587767	-1.679878
C	1.879961	2.950384	-0.326073
C	3.065261	3.170128	0.416913
C	3.657646	4.431944	0.403585
H	4.572675	4.597430	0.963525
C	3.092897	5.484600	-0.306008
H	3.569933	6.459833	-0.314434
C	1.904020	5.279725	-0.985326
H	1.448540	6.106023	-1.524517
C	1.275236	4.029580	-1.000374
C	3.638871	2.086315	1.310291
H	3.404407	1.120209	0.857263
C	5.156820	2.164739	1.496276
H	5.685886	2.261405	0.542846
H	5.512949	1.258444	1.996972
H	5.441557	3.013798	2.127275
C	2.949795	2.154794	2.682089
H	3.362637	1.406571	3.367371

H	1.870325	1.988634	2.595655
H	3.101022	3.145756	3.126593
C	-0.039144	3.911422	-1.750583
H	-0.436404	2.906162	-1.583024
C	0.163653	4.085484	-3.260083
H	-0.795812	4.032463	-3.787601
H	0.820615	3.307997	-3.664135
H	0.613436	5.059111	-3.484208
C	-1.058631	4.924474	-1.214141
H	-1.197987	4.797943	-0.135398
H	-2.027432	4.798009	-1.708440
H	-0.729134	5.952534	-1.397905
C	-1.799035	0.386851	0.251014
C	-2.877989	0.949085	-2.869275
H	-3.504434	0.802281	-3.754058
C	-4.453499	-0.920205	-2.181830
H	-4.376220	-1.770197	-1.493612
C	-4.818840	-1.729177	1.387804
H	-5.067902	-1.491444	0.352111
C	-2.873368	-1.287997	2.939734
H	-3.529470	-1.965697	3.496341
C	-0.872609	2.601997	1.925306
C	-1.941057	2.415957	1.147770
C	-0.519424	3.558468	3.034814
H	0.463893	3.995416	2.817008
H	-1.228991	4.393220	3.086176
C	-0.460276	2.851628	4.392207
H	-1.455841	2.510415	4.694619
H	-0.076330	3.516823	5.171826
H	0.190043	1.970895	4.339344
C	-3.329893	2.961368	1.073217
H	-3.388400	3.722624	0.283188
H	-3.996882	2.143828	0.736080
C	-3.866963	3.548087	2.384026
H	-3.684180	2.864079	3.219050
H	-4.945025	3.731331	2.321864
H	-3.379729	4.497782	2.619863
C	-2.806417	-0.060365	-0.654327
C	-2.893654	-0.452098	0.629439
N	-3.231572	-0.141826	-1.945214
N	-3.467827	-1.198120	1.596599
C	-2.864300	0.061506	3.654444
H	-2.230436	0.772307	3.117058
H	-3.875289	0.476958	3.715687

H	-2.471692	-0.048591	4.670906
C	-1.482962	-1.915279	2.889605
H	-1.073329	-2.001401	3.901410
H	-1.518962	-2.913426	2.440096
H	-0.799549	-1.303645	2.291284
C	-4.852677	-3.249802	1.541779
H	-5.846640	-3.633381	1.290979
H	-4.116830	-3.716041	0.879828
H	-4.631380	-3.555400	2.569711
C	-5.850326	-1.031499	2.276536
H	-5.669959	-1.237302	3.337164
H	-5.814273	0.052178	2.124437
H	-6.857858	-1.384617	2.035237
C	-3.194874	2.321007	-2.279531
H	-2.997733	3.106357	-3.017297
H	-4.242366	2.389821	-1.968599
H	-2.567258	2.503994	-1.402521
C	-1.417774	0.849334	-3.309065
H	-1.238335	-0.085361	-3.847077
H	-1.163496	1.685923	-3.967513
H	-0.740503	0.878714	-2.445775
C	-4.509902	-1.503776	-3.593196
H	-3.561742	-1.978813	-3.858265
H	-5.301045	-2.257989	-3.639969
H	-4.742439	-0.745473	-4.346811
C	-5.720846	-0.122742	-1.860665
H	-5.858907	0.682487	-2.591098
H	-6.608160	-0.763814	-1.895563
H	-5.655007	0.329961	-0.864685

INT7

Al	-0.383622	-0.728065	0.623988
P	-0.708610	1.835581	-0.148862
Si	-0.074472	4.327931	-0.391510
N	-2.052900	-0.932311	-0.304951
N	0.425676	2.787556	-1.051924
C	-1.958799	1.316732	-1.260125
C	-2.507172	0.064412	-1.116891
C	-3.708198	0.015155	-2.056662
H	-4.099705	-0.980764	-2.269659
C	-4.773573	1.024716	-1.521143
H	-5.695824	0.912145	-2.099219
H	-5.021596	0.851000	-0.473123

C	-4.123980	2.419192	-1.763497
H	-4.708550	3.005869	-2.480740
H	-4.017127	3.011965	-0.851295
C	-2.742124	2.034514	-2.347352
H	-2.204679	2.848877	-2.840769
C	-3.137762	0.835618	-3.234860
H	-3.899594	1.079121	-3.984782
H	-2.280056	0.360389	-3.719323
C	-0.984105	5.499850	-1.544782
H	-0.318076	5.960624	-2.281836
H	-1.439682	6.309628	-0.962048
H	-1.786192	4.981279	-2.078234
C	1.241638	5.338760	0.482980
H	1.815226	4.744641	1.197125
H	0.796272	6.188922	1.013006
H	1.940835	5.752619	-0.254184
N	-1.149254	3.345452	0.581070
C	-1.821104	3.554696	1.863404
C	-2.906926	2.496529	2.060782
H	-3.630468	2.513937	1.239011
H	-3.438489	2.662588	3.004171
H	-2.459012	1.497011	2.103689
C	-0.819197	3.464189	3.021801
H	-0.342425	2.476894	3.030606
H	-1.313266	3.618629	3.987587
H	-0.035385	4.221562	2.908419
C	-2.458119	4.946850	1.831503
H	-1.691739	5.722020	1.704175
H	-2.986672	5.153477	2.767803
H	-3.166734	5.021072	1.000239
C	1.344944	2.399293	-2.128185
C	0.987587	1.023604	-2.689443
H	1.037484	0.262468	-1.900830
H	1.719833	0.741888	-3.453542
H	-0.012204	1.014019	-3.134618
C	2.779306	2.343864	-1.588756
H	3.051128	3.297480	-1.119840
H	3.493098	2.138294	-2.396489
H	2.861654	1.546768	-0.841871
C	1.256612	3.448631	-3.241682
H	0.230594	3.527519	-3.616676
H	1.916293	3.182831	-4.074188
H	1.569005	4.435080	-2.874952
C	-2.916181	-2.059681	-0.095730

C	-4.031302	-1.940523	0.760557
C	-4.878477	-3.038219	0.925910
H	-5.740454	-2.953691	1.580853
C	-4.623310	-4.242619	0.285129
H	-5.286357	-5.090138	0.429122
C	-3.506015	-4.361460	-0.530824
H	-3.304869	-5.310822	-1.015407
C	-2.641233	-3.284386	-0.736767
C	-4.262203	-0.690169	1.589054
H	-3.814862	0.153941	1.058977
C	-5.740616	-0.367605	1.825346
H	-6.322542	-0.413515	0.899384
H	-5.836727	0.640069	2.244215
H	-6.193899	-1.059917	2.542887
C	-3.533204	-0.831592	2.932580
H	-3.716625	0.039911	3.571081
H	-2.452855	-0.935737	2.784842
H	-3.884743	-1.725678	3.461227
C	-1.460375	-3.421142	-1.681654
H	-0.630298	-2.839953	-1.259435
C	-1.817555	-2.827789	-3.051791
H	-1.029007	-3.024928	-3.784220
H	-1.959286	-1.745651	-2.990054
H	-2.746476	-3.276282	-3.422875
C	-0.969445	-4.859369	-1.846101
H	-0.763872	-5.329327	-0.878729
H	-0.046203	-4.864718	-2.433067
H	-1.697395	-5.476443	-2.384111
C	1.580257	-1.167567	0.508204
C	2.829921	-2.716999	-2.325856
H	3.638581	-3.012800	-3.003469
C	4.710528	-1.133026	-1.841171
H	4.843747	-0.225784	-1.241741
C	5.136895	0.183907	1.480938
H	5.343030	-0.631367	0.782092
C	3.091674	1.112618	2.610025
H	3.926588	1.515233	3.194215
C	-0.071692	-2.107520	1.991730
C	1.175691	-2.288901	1.484717
C	-0.643653	-2.983360	3.077846
H	0.163327	-3.489847	3.623618
H	-1.167519	-2.369966	3.822320
C	-1.613020	-4.048502	2.554197
H	-2.498898	-3.594528	2.103479

H	-1.941482	-4.710079	3.363082
H	-1.129252	-4.661094	1.784923
C	2.179817	-3.331755	1.929250
H	1.680096	-4.300513	2.051170
H	2.938665	-3.453437	1.149894
C	2.902086	-2.947749	3.227073
H	3.466712	-2.023610	3.077331
H	3.598033	-3.736552	3.532235
H	2.194391	-2.778630	4.044671
C	2.807859	-1.199132	-0.362497
C	2.921480	-0.508993	0.747629
N	3.329034	-1.546644	-1.595544
N	3.690642	0.127706	1.705479
C	2.115292	0.470386	3.595637
H	1.308456	-0.054969	3.073701
H	2.627868	-0.256251	4.231049
H	1.672118	1.239174	4.238147
C	2.441944	2.282240	1.875573
H	2.048015	3.006854	2.596026
H	3.158439	2.790325	1.224020
H	1.613442	1.930933	1.249760
C	5.613421	1.497141	0.850782
H	6.676780	1.437616	0.594674
H	5.049382	1.726955	-0.059127
H	5.486627	2.332177	1.549784
C	5.918264	-0.123314	2.761320
H	5.799920	0.663612	3.513327
H	5.586500	-1.069491	3.196928
H	6.986904	-0.199277	2.535829
C	2.531380	-3.922137	-1.436582
H	2.277655	-4.789457	-2.054797
H	3.402612	-4.181086	-0.827569
H	1.686416	-3.720376	-0.768274
C	1.623299	-2.346205	-3.183530
H	1.884834	-1.565079	-3.903297
H	1.255000	-3.219597	-3.733739
H	0.814404	-1.965447	-2.550707
C	4.928280	-0.734888	-3.301071
H	4.191057	0.015337	-3.602128
H	5.930539	-0.313847	-3.429778
H	4.843572	-1.591382	-3.978244
C	5.728930	-2.182629	-1.381756
H	5.687228	-3.072111	-2.021272
H	6.750122	-1.788908	-1.425160

H	5.518482	-2.495923	-0.353492

TS(INT7-->INT8)

Al	0.146629	0.243107	0.760412
P	2.544967	-0.127391	-0.013285
Si	4.598242	-1.699194	-0.020451
N	0.156584	1.799890	-0.344941
N	3.322572	-1.220557	-1.115895
C	2.596821	1.533266	-0.567078
C	1.392546	2.214330	-0.713257
C	1.735693	3.594311	-1.253250
H	0.912155	4.134769	-1.720271
C	2.393488	4.327031	-0.044168
H	2.511880	5.390007	-0.273376
H	1.775049	4.244622	0.855147
C	3.769389	3.614776	0.098342
H	4.592427	4.305954	-0.112467
H	3.923398	3.196658	1.094146
C	3.692029	2.503712	-0.985027
H	4.653359	2.046233	-1.231475
C	2.970601	3.272243	-2.112902
H	3.502992	4.173178	-2.438375
H	2.732283	2.648673	-2.980660
C	6.355990	-1.261337	-0.509450
H	6.696328	-1.847598	-1.370799
H	7.043671	-1.468742	0.318420
H	6.436454	-0.199402	-0.760216
C	4.543192	-3.508046	0.474438
H	3.521221	-3.807014	0.725420
H	5.185904	-3.723851	1.335021
H	4.887257	-4.138082	-0.353974
N	3.829324	-0.557649	1.063648
C	3.863694	-0.489758	2.529508
C	3.462807	0.915887	2.974068
H	4.182869	1.644363	2.589079
H	3.436054	0.989795	4.066681
H	2.469137	1.173661	2.595374
C	2.949281	-1.557264	3.143930
H	1.914326	-1.424803	2.809621
H	2.965750	-1.507081	4.238808
H	3.285418	-2.556452	2.845710
C	5.311450	-0.748574	2.961368
H	5.635277	-1.758992	2.681296

H	5.402751	-0.665647	4.048978
H	5.986194	-0.022729	2.496004
C	3.226904	-1.323765	-2.573474
C	1.789371	-1.071575	-3.010791
H	1.112148	-1.796398	-2.553451
H	1.694598	-1.142156	-4.100249
H	1.477785	-0.069432	-2.705063
C	3.642314	-2.746515	-2.961734
H	4.691152	-2.935869	-2.698236
H	3.541203	-2.897854	-4.041339
H	3.018751	-3.479741	-2.439557
C	4.154106	-0.312454	-3.261290
H	3.863860	0.707592	-2.994486
H	4.101828	-0.414342	-4.351159
H	5.193540	-0.467329	-2.952951
C	-0.979713	2.552656	-0.795908
C	-1.767671	3.278702	0.115714
C	-2.831713	4.045948	-0.374235
H	-3.444434	4.604959	0.327871
C	-3.110812	4.114388	-1.729303
H	-3.928372	4.730163	-2.091489
C	-2.350363	3.364029	-2.620854
H	-2.592049	3.390099	-3.678621
C	-1.303964	2.560235	-2.174064
C	-1.545777	3.219688	1.614028
H	-0.605628	2.694328	1.799345
C	-1.430873	4.613989	2.239436
H	-0.646544	5.202751	1.752943
H	-1.188959	4.534971	3.304161
H	-2.369800	5.172078	2.157747
C	-2.676016	2.407604	2.264754
H	-2.486926	2.254535	3.332906
H	-2.778024	1.419861	1.798344
H	-3.629820	2.940225	2.162565
C	-0.596209	1.622275	-3.135021
H	0.454791	1.562436	-2.838729
C	-0.616195	2.079724	-4.593932
H	0.031500	1.429694	-5.191226
H	-0.258516	3.109395	-4.697121
H	-1.621061	2.021036	-5.025640
C	-1.220429	0.221968	-3.006113
H	-1.154578	-0.166556	-1.981162
H	-0.732087	-0.490769	-3.679697
H	-2.282045	0.268302	-3.274945

C	-1.315221	-1.050570	0.983085
C	-0.661104	-3.235124	-0.959834
H	-0.070202	-2.313177	-0.928699
C	-3.218073	-3.613113	-1.050965
H	-4.038236	-3.110182	-0.529118
C	-4.571866	-0.516163	-0.964822
H	-3.738706	-1.056261	-1.425019
C	-5.345968	-0.303963	1.505550
H	-4.736052	-0.160057	2.403124
C	-0.124714	0.131680	2.684927
C	-1.043597	-0.858789	2.438139
C	0.277718	0.564550	4.069545
H	-0.448023	0.204525	4.813020
H	1.232470	0.096405	4.350327
C	0.426508	2.078882	4.249742
H	1.064558	2.518171	3.474152
H	0.865844	2.318285	5.224264
H	-0.545555	2.575485	4.190936
C	-1.682350	-1.722507	3.506165
H	-2.153601	-1.077359	4.259476
H	-2.487116	-2.309367	3.059018
C	-0.655626	-2.637075	4.183035
H	-0.172239	-3.287424	3.445639
H	-1.132135	-3.276378	4.933530
H	0.133833	-2.062629	4.677968
C	-2.217656	-1.934788	0.351218
C	-3.265685	-1.329489	0.961019
N	-2.043085	-2.787371	-0.729091
N	-4.359551	-0.714054	0.484137
C	-6.333455	-1.436258	1.802774
H	-7.013310	-1.612473	0.963248
H	-5.779888	-2.358497	2.004625
H	-6.939661	-1.195311	2.682652
C	-6.071520	1.011995	1.232772
H	-6.657851	1.273390	2.119531
H	-5.365570	1.823241	1.038235
H	-6.768070	0.943234	0.391612
C	-5.870251	-1.132010	-1.491064
H	-5.880387	-1.081767	-2.585527
H	-5.965427	-2.182095	-1.195969
H	-6.752675	-0.595158	-1.129526
C	-4.418125	0.940773	-1.408580
H	-5.285723	1.556777	-1.162924
H	-3.530732	1.384104	-0.946260

H	-4.291138	0.980809	-2.496295
C	-0.098770	-4.141898	0.143455
H	0.988727	-4.218860	0.028754
H	-0.308564	-3.713355	1.127905
H	-0.514401	-5.152324	0.102060
C	-0.460746	-3.852162	-2.339704
H	-0.826341	-3.188246	-3.129309
H	0.607496	-4.028030	-2.503283
H	-0.964341	-4.818788	-2.433198
C	-3.161094	-5.033897	-0.480169
H	-2.928862	-5.009456	0.588715
H	-4.133118	-5.520649	-0.611674
H	-2.413251	-5.651193	-0.987320
C	-3.587930	-3.622723	-2.539016
H	-2.958554	-4.298030	-3.123488
H	-4.624140	-3.959445	-2.653599
H	-3.502992	-2.618967	-2.967238

INT8

Al	0.150268	0.139825	0.487808
P	2.537362	-0.521519	-0.031596
Si	4.488076	-2.066996	0.609307
N	0.535819	1.663206	-0.630944
N	3.252879	-1.963416	-0.628138
C	2.735134	0.756170	-1.194592
C	1.724461	1.689772	-1.281065
C	2.241653	2.796586	-2.185259
H	1.487401	3.473925	-2.587828
C	3.373188	3.505818	-1.372384
H	3.671422	4.427164	-1.881642
H	3.036422	3.778078	-0.367413
C	4.527316	2.461702	-1.361010
H	5.391567	2.828884	-1.925209
H	4.867636	2.203270	-0.355018
C	3.877390	1.244249	-2.067568
H	4.579618	0.469867	-2.387174
C	3.076726	1.961888	-3.177012
H	3.698010	2.582958	-3.832566
H	2.466469	1.278128	-3.775414
C	6.253208	-1.977994	-0.010775
H	6.539667	-2.894014	-0.539079
H	6.956507	-1.840535	0.818186
H	6.366488	-1.133591	-0.697417

C	4.311761	-3.509782	1.794990
H	3.288840	-3.571076	2.180433
H	4.996254	-3.417632	2.646135
H	4.546347	-4.455945	1.292731
N	3.812186	-0.536641	1.133545
C	3.862797	0.196842	2.401616
C	3.193399	1.567258	2.247195
H	3.651683	2.140917	1.434941
H	3.289729	2.137816	3.177294
H	2.121123	1.461873	2.038852
C	3.146751	-0.601479	3.497528
H	2.130926	-0.839528	3.166257
H	3.083361	-0.033659	4.432650
H	3.675755	-1.539307	3.699504
C	5.337859	0.385362	2.765889
H	5.835362	-0.586702	2.878321
H	5.437031	0.920548	3.715940
H	5.856687	0.948763	1.983701
C	2.701492	-2.902247	-1.602571
C	1.987102	-2.143391	-2.726055
H	1.128604	-1.577335	-2.342473
H	1.614534	-2.849113	-3.476214
H	2.668927	-1.436458	-3.210026
C	1.721541	-3.854382	-0.911289
H	2.237141	-4.448427	-0.148210
H	1.268822	-4.541694	-1.635146
H	0.923601	-3.284895	-0.418692
C	3.871601	-3.695106	-2.191581
H	4.587028	-3.020171	-2.672600
H	3.514529	-4.418438	-2.931549
H	4.395217	-4.255466	-1.406173
C	-0.414223	2.692155	-0.924403
C	-0.530889	3.803840	-0.067249
C	-1.545873	4.733055	-0.306396
H	-1.659573	5.580751	0.364211
C	-2.408894	4.591456	-1.386423
H	-3.201290	5.315150	-1.551696
C	-2.224855	3.540003	-2.277010
H	-2.862727	3.461343	-3.154154
C	-1.214986	2.594611	-2.079259
C	0.428375	4.017501	1.088216
H	1.245498	3.299083	0.970766
C	1.034658	5.424611	1.077206
H	1.483374	5.659275	0.106394

H	1.811759	5.503929	1.844984
H	0.280974	6.189582	1.292891
C	-0.259561	3.714969	2.419619
H	0.437299	3.825742	3.259062
H	-0.631951	2.687974	2.410439
H	-1.106997	4.391910	2.584770
C	-0.962626	1.539801	-3.143377
H	-0.082192	0.958625	-2.851172
C	-0.660200	2.189548	-4.500394
H	-0.397307	1.421254	-5.235150
H	0.172425	2.896886	-4.432777
H	-1.531141	2.732151	-4.883941
C	-2.136369	0.569392	-3.255847
H	-2.251987	-0.023085	-2.341906
H	-1.981086	-0.127947	-4.087825
H	-3.072898	1.109465	-3.445547
C	-1.307818	-1.190730	0.582146
C	-1.729473	-3.040083	-1.662795
H	-0.791727	-2.509281	-1.485831
C	-4.185923	-2.296204	-1.565326
H	-4.726992	-1.565262	-0.961333
C	-4.143153	0.693015	0.390455
H	-3.465308	0.376121	-0.405186
C	-5.447433	-0.642219	2.207681
H	-5.116299	-1.469853	2.837985
C	-0.329160	0.106092	2.371262
C	-1.091310	-0.988922	2.048461
C	-0.050896	0.484987	3.807760
H	0.307735	-0.383758	4.381901
H	0.753531	1.229544	3.867298
C	-1.287249	1.043411	4.531081
H	-1.652506	1.956939	4.052968
H	-1.060685	1.276800	5.577146
H	-2.107286	0.318449	4.513559
C	-1.434583	-2.101280	3.029762
H	-1.607479	-1.693627	4.031181
H	-2.348833	-2.615350	2.723600
C	-0.269207	-3.100189	3.088168
H	-0.045058	-3.478366	2.084638
H	-0.507741	-3.953729	3.730916
H	0.637292	-2.622306	3.476906
C	-2.523599	-1.604967	0.101950
C	-3.651442	-1.651872	1.047877
N	-2.767543	-2.088913	-1.204894

N	-4.351838	-0.557154	1.198605
C	-6.768095	-1.065297	1.564531
H	-7.217351	-0.272106	0.962125
H	-6.604273	-1.944059	0.932446
H	-7.483176	-1.336269	2.347815
C	-5.594398	0.592263	3.091597
H	-6.294256	0.353560	3.898461
H	-4.638531	0.873146	3.541818
H	-5.997090	1.455063	2.554235
C	-5.409659	1.207598	-0.290023
H	-5.115560	2.009487	-0.975840
H	-5.906670	0.426634	-0.874801
H	-6.130399	1.627635	0.417269
C	-3.416624	1.796187	1.159641
H	-4.078166	2.352780	1.829015
H	-2.586762	1.377421	1.737871
H	-3.002461	2.506024	0.434727
C	-1.694097	-4.329013	-0.827723
H	-0.795113	-4.906534	-1.059663
H	-1.681173	-4.089189	0.240344
H	-2.554360	-4.969543	-1.030601
C	-1.780062	-3.362799	-3.151591
H	-1.844194	-2.456076	-3.759311
H	-0.860833	-3.894775	-3.421088
H	-2.618332	-4.019241	-3.405690
C	-4.774698	-3.666721	-1.204242
H	-4.526229	-3.932690	-0.173278
H	-5.865852	-3.625210	-1.298774
H	-4.419652	-4.452037	-1.879234
C	-4.538531	-1.928999	-3.011886
H	-4.203578	-2.671640	-3.738019
H	-5.629305	-1.865288	-3.095497
H	-4.120841	-0.959069	-3.286784

TS(INT8-->INT9)

Al	0.078482	0.420268	0.581419
P	2.335739	-0.612847	0.065498
Si	3.871694	-2.657357	0.399239
N	0.693403	1.832561	-0.546105
N	2.663891	-2.103512	-0.739777
C	2.863942	0.747586	-0.897334
C	1.931136	1.752539	-1.086158
C	2.591284	2.805964	-1.960968

H	1.912267	3.503891	-2.452207
C	3.660897	3.479640	-1.049915
H	4.059489	4.373857	-1.537971
H	3.231931	3.785227	-0.090844
C	4.747078	2.377181	-0.896394
H	5.686628	2.682540	-1.369681
H	4.957682	2.150578	0.150131
C	4.116950	1.170876	-1.649049
H	4.814841	0.364053	-1.887312
C	3.480860	1.912031	-2.846522
H	4.201223	2.489513	-3.437660
H	2.904680	1.252881	-3.503275
C	5.613190	-2.796851	-0.290631
H	5.672421	-3.604148	-1.029513
H	6.340583	-3.022271	0.497410
H	5.914344	-1.864683	-0.778233
C	3.485091	-4.247999	1.312777
H	2.498583	-4.206255	1.781963
H	4.229835	-4.443555	2.092398
H	3.506339	-5.102689	0.625694
N	3.492743	-1.160547	1.222270
C	4.100363	-0.434023	2.340874
C	3.315167	0.850962	2.613713
H	3.357296	1.533796	1.756728
H	3.728761	1.367738	3.485449
H	2.265228	0.617924	2.820715
C	4.055240	-1.326588	3.586429
H	3.020575	-1.554200	3.859248
H	4.543020	-0.834014	4.434525
H	4.577885	-2.273092	3.401124
C	5.561922	-0.104041	2.009814
H	6.154514	-1.021957	1.924115
H	6.012870	0.516530	2.791997
H	5.625633	0.427182	1.055907
C	1.930274	-2.736064	-1.835468
C	1.244389	-1.676021	-2.704026
H	0.511232	-1.102904	-2.120440
H	0.708842	-2.161191	-3.528871
H	1.977114	-0.977254	-3.120912
C	0.875620	-3.706352	-1.288964
H	1.343600	-4.456234	-0.641100
H	0.368317	-4.229179	-2.108205
H	0.126290	-3.162844	-0.701667
C	2.944295	-3.510469	-2.684725

H	3.722940	-2.836002	-3.054826
H	2.452721	-3.988940	-3.538237
H	3.422959	-4.300573	-2.091821
C	-0.180379	2.886956	-0.951351
C	-0.504454	3.907718	-0.037665
C	-1.448766	4.865321	-0.419362
H	-1.718966	5.651072	0.281657
C	-2.032028	4.841535	-1.679103
H	-2.762939	5.594943	-1.956713
C	-1.665526	3.855480	-2.589029
H	-2.118962	3.843683	-3.576832
C	-0.745670	2.865727	-2.244312
C	0.178575	4.036252	1.314254
H	0.884679	3.203993	1.415201
C	0.975412	5.346616	1.382249
H	1.669510	5.438898	0.540600
H	1.549313	5.396740	2.313573
H	0.305314	6.213317	1.356455
C	-0.817607	3.942289	2.473653
H	-0.298860	4.062771	3.431974
H	-1.302779	2.961098	2.464189
H	-1.580355	4.727437	2.405408
C	-0.420100	1.759439	-3.235477
H	0.469698	1.228610	-2.885040
C	-0.104644	2.290805	-4.636917
H	0.214649	1.468237	-5.285823
H	0.697432	3.035714	-4.609399
H	-0.980217	2.755015	-5.102979
C	-1.561537	0.737102	-3.279584
H	-1.749090	0.320867	-2.281773
H	-1.313152	-0.089114	-3.957185
H	-2.487474	1.205437	-3.636958
C	-1.249894	-0.967551	0.051630
C	-2.585683	-2.846032	-2.131668
H	-1.581075	-2.405897	-2.134753
C	-4.319638	-3.085717	-0.190947
H	-4.587444	-2.370426	0.595999
C	-4.213335	0.541697	-0.137566
H	-3.836489	-0.158484	-0.891231
C	-4.043600	0.573913	2.443340
H	-3.176967	0.397476	3.083124
C	-0.705150	0.403984	2.290919
C	-1.396404	-0.833074	1.974206
C	-0.180366	0.646652	3.690003

H	0.449086	-0.178094	4.081593
H	0.480752	1.524248	3.673466
C	-1.262243	0.917546	4.746578
H	-1.879975	1.774159	4.452912
H	-0.824357	1.128607	5.729601
H	-1.928250	0.053094	4.861497
C	-1.062322	-2.138276	2.695708
H	-1.278041	-1.979234	3.761774
H	-1.734147	-2.935692	2.359127
C	0.392917	-2.565957	2.523270
H	0.591759	-2.806906	1.471595
H	0.625747	-3.448199	3.129471
H	1.078494	-1.761495	2.802798
C	-2.341827	-1.750666	0.013514
C	-2.606444	-0.855666	1.132052
N	-3.105870	-2.512864	-0.798492
N	-3.628258	0.091246	1.125119
C	-5.213223	-0.233814	3.020942
H	-6.146775	-0.050584	2.480286
H	-4.989866	-1.305349	2.973051
H	-5.375587	0.032958	4.071348
C	-4.305810	2.076729	2.514732
H	-4.441426	2.361602	3.563614
H	-3.456197	2.634116	2.112995
H	-5.211916	2.372192	1.975830
C	-5.741035	0.432879	-0.171825
H	-6.101216	0.645287	-1.184456
H	-6.076243	-0.569673	0.112866
H	-6.214331	1.154325	0.501142
C	-3.750978	1.935902	-0.580974
H	-4.274419	2.736654	-0.052120
H	-2.677034	2.056512	-0.406076
H	-3.939835	2.068237	-1.652528
C	-2.439132	-4.350219	-2.361952
H	-1.899840	-4.524235	-3.299276
H	-1.880777	-4.820998	-1.548233
H	-3.413023	-4.842489	-2.448682
C	-3.364367	-2.186187	-3.276752
H	-3.573430	-1.136221	-3.052677
H	-2.763650	-2.224750	-4.191857
H	-4.309239	-2.695714	-3.480311
C	-4.064018	-4.435178	0.488393
H	-3.186893	-4.372476	1.139150
H	-4.927700	-4.712045	1.101863

H	-3.899189	-5.233921	-0.240012
C	-5.504045	-3.158151	-1.151151
H	-5.361309	-3.917175	-1.926400
H	-6.399837	-3.433167	-0.585752
H	-5.685525	-2.193219	-1.632652

INT9

Al	0.100155	0.230586	0.416584
P	2.375639	-0.679462	-0.077993
Si	3.722502	-2.819370	0.382211
N	0.782793	1.838718	-0.388752
N	2.668605	-2.178742	-0.867959
C	2.894603	0.723445	-0.968277
C	1.978231	1.768286	-1.007698
C	2.611799	2.869970	-1.838694
H	1.923529	3.629043	-2.209002
C	3.768718	3.435843	-0.961284
H	4.144496	4.367994	-1.392854
H	3.425757	3.654806	0.055288
C	4.837393	2.309459	-1.005721
H	5.723984	2.633851	-1.561260
H	5.164842	2.008139	-0.010290
C	4.103486	1.176274	-1.777814
H	4.751448	0.371397	-2.133545
C	3.396326	2.024135	-2.860890
H	4.085272	2.625061	-3.465716
H	2.747935	1.429771	-3.511565
C	5.448884	-3.262621	-0.200284
H	5.406240	-4.140841	-0.855000
H	6.111404	-3.511078	0.636350
H	5.895243	-2.438744	-0.764662
C	3.039113	-4.239969	1.397298
H	2.053222	-3.981481	1.796643
H	3.700728	-4.459896	2.242980
H	2.945951	-5.160234	0.809387
N	3.491945	-1.244845	1.116528
C	4.299052	-0.482403	2.077430
C	3.654773	0.878978	2.357031
H	3.682233	1.526266	1.475971
H	4.183751	1.382741	3.172519
H	2.610440	0.754157	2.655249
C	4.377820	-1.285863	3.380659
H	3.385357	-1.414537	3.821803

H	5.024025	-0.780501	4.106451
H	4.801258	-2.280816	3.192876
C	5.721171	-0.285411	1.529921
H	6.265050	-1.235789	1.511269
H	6.289571	0.414773	2.152454
H	5.684662	0.101550	0.507787
C	1.778951	-2.839594	-1.829491
C	1.247292	-1.814557	-2.837803
H	0.575423	-1.093083	-2.354422
H	0.674409	-2.323121	-3.621913
H	2.073769	-1.265681	-3.302041
C	0.605692	-3.522111	-1.116687
H	0.968012	-4.276190	-0.410344
H	-0.039068	-4.023082	-1.845172
H	-0.001307	-2.791482	-0.567923
C	2.616951	-3.890576	-2.563586
H	3.469941	-3.419003	-3.061349
H	2.012649	-4.412857	-3.312218
H	2.997571	-4.643761	-1.861210
C	-0.126980	2.882552	-0.749889
C	-0.425881	3.872969	0.204163
C	-1.387774	4.837699	-0.106887
H	-1.633986	5.600302	0.628081
C	-2.036364	4.831710	-1.334060
H	-2.792510	5.578194	-1.556676
C	-1.696864	3.876341	-2.285899
H	-2.190091	3.889119	-3.254736
C	-0.737106	2.896721	-2.025819
C	0.306335	3.949138	1.534177
H	1.034502	3.130714	1.561589
C	1.079747	5.269298	1.647679
H	1.750855	5.409676	0.794230
H	1.677030	5.285932	2.565449
H	0.396046	6.124928	1.678327
C	-0.645770	3.775177	2.720893
H	-0.099106	3.852457	3.667178
H	-1.136256	2.795816	2.689616
H	-1.423435	4.547360	2.715764
C	-0.361513	1.925966	-3.140286
H	0.439132	1.273082	-2.777726
C	0.161640	2.674875	-4.375415
H	0.512034	1.959154	-5.127103
H	0.989098	3.348881	-4.135494
H	-0.633520	3.272566	-4.834256

C	-1.528490	1.018026	-3.542582
H	-1.831470	0.402859	-2.692400
H	-1.224947	0.360330	-4.366387
H	-2.391615	1.604686	-3.880181
C	-1.534393	-0.392466	-0.386177
C	-2.623292	-2.717356	-2.228888
H	-1.615595	-2.308569	-2.374001
C	-3.899343	-3.289478	-0.034438
H	-3.975169	-2.728342	0.904944
C	-4.587257	0.320702	-0.057757
H	-4.465320	-0.633984	-0.575450
C	-3.734522	1.263912	2.136385
H	-2.797125	1.143073	2.687463
C	-0.425151	-0.306414	2.259419
C	-1.694839	-0.765577	2.194945
C	0.413917	-0.481606	3.503700
H	-0.009538	-1.234502	4.180160
H	1.405300	-0.858876	3.219822
C	0.564590	0.829809	4.281185
H	0.947716	1.629665	3.637837
H	1.244910	0.719851	5.132980
H	-0.410078	1.160563	4.657030
C	-2.411021	-1.520818	3.297029
H	-2.208140	-1.079463	4.280918
H	-3.489893	-1.442963	3.129213
C	-2.010627	-3.001428	3.296494
H	-2.180091	-3.436091	2.306899
H	-2.590091	-3.575684	4.026701
H	-0.947707	-3.122486	3.527034
C	-2.351520	-1.430133	-0.229385
C	-2.473457	-0.534261	0.907117
N	-2.870171	-2.559733	-0.788769
N	-3.722751	0.204236	1.117154
C	-4.861714	1.096531	3.170162
H	-5.835865	1.390347	2.770446
H	-4.934067	0.061594	3.512749
H	-4.660633	1.733258	4.039250
C	-3.739007	2.704891	1.612192
H	-3.568387	3.394987	2.445972
H	-2.955402	2.866816	0.866583
H	-4.703806	2.968285	1.167173
C	-6.072895	0.410362	0.298315
H	-6.672926	0.260237	-0.606656
H	-6.345784	-0.354373	1.032276

H	-6.339791	1.392143	0.701418
C	-4.222223	1.404743	-1.095406
H	-4.636302	2.385113	-0.846006
H	-3.138139	1.503292	-1.189941
H	-4.628639	1.123480	-2.075519
C	-2.613314	-4.170477	-2.698826
H	-2.233541	-4.209636	-3.725165
H	-1.977843	-4.798151	-2.070170
H	-3.618806	-4.602350	-2.708207
C	-3.578038	-1.874066	-3.084063
H	-3.621922	-0.849175	-2.705783
H	-3.220181	-1.837433	-4.119009
H	-4.589639	-2.290666	-3.090482
C	-3.471796	-4.723979	0.310337
H	-2.411452	-4.759176	0.575268
H	-4.055338	-5.091307	1.161153
H	-3.639361	-5.409256	-0.525541
C	-5.294716	-3.298094	-0.669702
H	-5.316623	-3.880798	-1.595538
H	-5.997455	-3.767015	0.026958
H	-5.655118	-2.289131	-0.885576

TS(INT9-->INT10)

Al	1.412269	-0.296210	0.310275
P	-2.437240	0.014434	-0.120385
Si	-4.825813	0.643992	0.690054
N	0.546740	-1.899298	-0.046122
N	-4.111997	-0.321571	-0.570836
C	-1.909986	-1.611122	0.504370
C	-0.721329	-2.276926	0.396575
C	-0.932189	-3.661079	1.017073
H	-0.196723	-4.412058	0.725869
C	-1.043143	-3.409097	2.552716
H	-1.017019	-4.357297	3.100065
H	-0.218064	-2.789123	2.919928
C	-2.424124	-2.705639	2.684699
H	-3.128656	-3.328296	3.247549
H	-2.369675	-1.731573	3.174349
C	-2.871763	-2.570770	1.206145
H	-3.925167	-2.321715	1.064714
C	-2.396594	-3.924398	0.649942
H	-2.825094	-4.788305	1.171921
H	-2.548646	-4.027094	-0.428707

C	-6.076309	-0.202671	1.805919
H	-6.979143	-0.478214	1.248644
H	-6.382366	0.459208	2.624340
H	-5.650387	-1.110683	2.243119
C	-5.593503	2.266532	0.104164
H	-4.899769	2.806805	-0.548342
H	-5.848666	2.921970	0.945003
H	-6.519236	2.092200	-0.457090
N	-3.198673	0.757454	1.301023
C	-2.573997	1.732651	2.191874
C	-1.323001	1.125056	2.828710
H	-1.576280	0.220249	3.389627
H	-0.843481	1.838943	3.508922
H	-0.591389	0.860657	2.059883
C	-2.188582	3.015264	1.436555
H	-1.493343	2.772973	0.624571
H	-1.703416	3.738010	2.104836
H	-3.079255	3.487329	1.005925
C	-3.582115	2.066226	3.296301
H	-4.482291	2.536667	2.881481
H	-3.146145	2.764719	4.018226
H	-3.878364	1.153998	3.825039
C	-4.559945	-0.656471	-1.919801
C	-3.823571	-1.908270	-2.404171
H	-2.745887	-1.719291	-2.449067
H	-4.162938	-2.199342	-3.404856
H	-3.994823	-2.739823	-1.712822
C	-4.304102	0.498762	-2.899592
H	-4.856778	1.391678	-2.587752
H	-4.618620	0.234990	-3.915821
H	-3.236832	0.746063	-2.919120
C	-6.060586	-0.955316	-1.852983
H	-6.252356	-1.768882	-1.145433
H	-6.442353	-1.247357	-2.836866
H	-6.622498	-0.071229	-1.527206
C	1.333788	-2.924116	-0.673107
C	2.398760	-3.537448	0.017442
C	3.261826	-4.382382	-0.690460
H	4.100297	-4.841505	-0.171629
C	3.042669	-4.668827	-2.029341
H	3.722638	-5.322338	-2.567155
C	1.914444	-4.157922	-2.667300
H	1.716107	-4.437924	-3.696924
C	1.041825	-3.293179	-2.007845

C	2.547582	-3.422291	1.527675
H	1.748639	-2.763713	1.881839
C	2.348787	-4.793716	2.190611
H	1.408822	-5.260867	1.885031
H	2.338494	-4.686067	3.280725
H	3.164670	-5.476354	1.927684
C	3.887015	-2.831623	1.972863
H	3.964441	-2.842144	3.066143
H	3.997005	-1.797448	1.639441
H	4.728855	-3.406764	1.570037
C	-0.212819	-2.766446	-2.692449
H	-1.000318	-2.753018	-1.932123
C	-0.700580	-3.665200	-3.830651
H	-1.691539	-3.334294	-4.158270
H	-0.774985	-4.711331	-3.517400
H	-0.036682	-3.614334	-4.701155
C	-0.053060	-1.327450	-3.199500
H	0.187188	-0.637164	-2.384804
H	-0.986424	-0.984183	-3.661073
H	0.735401	-1.275409	-3.958226
C	0.645858	1.453295	-0.276655
C	-0.123254	3.933928	-2.098748
H	-0.679250	3.008112	-1.910696
C	1.920198	4.930591	-0.782767
H	2.820080	4.424474	-0.409513
C	2.964046	0.653111	-2.032878
H	1.903800	0.884035	-2.206352
C	4.380290	0.287470	0.042152
H	4.158156	0.014196	1.074999
C	1.961438	0.370686	2.122618
C	2.284068	1.633308	1.760609
C	2.100367	-0.227903	3.501314
H	1.246242	0.106464	4.110638
H	1.984323	-1.315826	3.431882
C	3.406454	0.062509	4.251557
H	4.274414	-0.128212	3.609903
H	3.493018	-0.581509	5.132332
H	3.466425	1.098062	4.596617
C	2.820414	2.797333	2.570908
H	3.773898	2.532682	3.042041
H	3.036605	3.634075	1.894477
C	1.821120	3.263052	3.633837
H	0.877768	3.563591	3.164962
H	2.211042	4.113650	4.201449

H	1.592210	2.457119	4.338582
C	1.161243	2.669750	-0.530938
C	1.919603	1.880464	0.329146
N	1.043199	3.828522	-1.202362
N	3.047703	0.427098	-0.579891
C	5.188632	1.591097	0.155169
H	5.707915	1.854886	-0.768460
H	4.547001	2.430223	0.441399
H	5.950386	1.467247	0.933144
C	5.259608	-0.829114	-0.532313
H	6.061790	-1.058474	0.178486
H	4.685100	-1.744462	-0.709077
H	5.733083	-0.526462	-1.471282
C	3.754474	1.858283	-2.555292
H	3.407316	2.101864	-3.565479
H	3.610534	2.739626	-1.921557
H	4.825398	1.645498	-2.624269
C	3.266238	-0.578257	-2.899009
H	4.338195	-0.766394	-2.985930
H	2.792532	-1.478256	-2.498300
H	2.881201	-0.410217	-3.910852
C	-1.054588	5.095807	-1.756133
H	-1.955831	5.025437	-2.372937
H	-1.355491	5.058908	-0.705235
H	-0.593780	6.068027	-1.957035
C	0.275881	3.928499	-3.576317
H	0.975358	3.110799	-3.774757
H	-0.613401	3.778131	-4.196655
H	0.742114	4.868740	-3.882189
C	1.340097	5.739116	0.382400
H	0.976155	5.066170	1.166385
H	2.113804	6.382943	0.813742
H	0.510936	6.375697	0.062398
C	2.357731	5.821429	-1.941478
H	1.524481	6.397551	-2.354116
H	3.104042	6.535512	-1.580926
H	2.805241	5.228163	-2.743808

INT10

Al	1.278934	0.766334	0.463705
P	-1.622788	-1.313116	0.056892
Si	-3.869216	-2.557678	-0.328698
N	1.829480	-0.914932	-0.192626

N	-2.577276	-1.923875	-1.302634
C	-0.199260	-2.401927	0.026841
C	1.131254	-2.109293	-0.157511
C	1.848002	-3.465850	-0.247446
H	2.847172	-3.443878	-0.683700
C	1.795725	-4.078476	1.187058
H	2.438453	-4.963538	1.240177
H	2.141139	-3.371219	1.944703
C	0.297105	-4.444950	1.360800
H	0.162450	-5.528204	1.455652
H	-0.149745	-3.969880	2.234391
C	-0.322132	-3.923311	0.040220
H	-1.328445	-4.291707	-0.165188
C	0.778856	-4.314602	-0.955099
H	1.018653	-5.385192	-0.955820
H	0.558097	-3.981067	-1.972241
C	-4.323821	-4.364988	-0.555454
H	-4.827327	-4.520270	-1.516798
H	-5.012853	-4.689942	0.233033
H	-3.442177	-5.010166	-0.524232
C	-5.487914	-1.589367	-0.438746
H	-5.317580	-0.513123	-0.335487
H	-6.207506	-1.897580	0.328490
H	-5.966077	-1.761083	-1.411375
N	-2.824804	-2.180349	1.024016
C	-3.172548	-1.823080	2.399632
C	-1.931323	-1.938799	3.287281
H	-1.569357	-2.969856	3.292093
H	-2.161331	-1.648561	4.319270
H	-1.128577	-1.290983	2.914686
C	-3.733952	-0.394068	2.481771
H	-2.992712	0.317731	2.097532
H	-3.979775	-0.118331	3.514013
H	-4.644172	-0.305626	1.879133
C	-4.228458	-2.818904	2.889122
H	-5.149208	-2.739560	2.298171
H	-4.488234	-2.625182	3.935184
H	-3.848446	-3.841937	2.804079
C	-2.535022	-1.351970	-2.643716
C	-1.077716	-1.154965	-3.067304
H	-0.596469	-0.404076	-2.427138
H	-1.016974	-0.805745	-4.104893
H	-0.520774	-2.092229	-2.970246
C	-3.245117	0.009819	-2.689730

H	-4.318231	-0.098807	-2.495898
H	-3.119983	0.490305	-3.668221
H	-2.820974	0.668194	-1.920265
C	-3.224920	-2.331430	-3.596244
H	-2.717518	-3.300708	-3.571007
H	-3.215877	-1.951290	-4.623488
H	-4.272502	-2.482084	-3.304898
C	3.198386	-1.002318	-0.648690
C	4.247972	-1.114170	0.287096
C	5.567129	-1.178845	-0.168828
H	6.374646	-1.255233	0.554807
C	5.863084	-1.162402	-1.524777
H	6.893173	-1.219024	-1.863042
C	4.825309	-1.083025	-2.442977
H	5.050362	-1.087260	-3.506602
C	3.493761	-0.998058	-2.030418
C	3.993221	-1.203587	1.780545
H	2.913915	-1.323135	1.919380
C	4.688562	-2.419848	2.405319
H	4.476981	-3.335298	1.844937
H	4.350129	-2.560440	3.437793
H	5.775253	-2.284626	2.431582
C	4.426465	0.081305	2.493893
H	4.242578	0.009126	3.572481
H	3.886336	0.944470	2.093435
H	5.498229	0.259675	2.344398
C	2.404983	-0.981453	-3.088863
H	1.458382	-0.790804	-2.578788
C	2.318755	-2.352902	-3.773129
H	1.471527	-2.387869	-4.467345
H	2.202863	-3.157485	-3.042761
H	3.232783	-2.551756	-4.345102
C	2.602672	0.101967	-4.156219
H	2.670072	1.103904	-3.723507
H	1.758320	0.090403	-4.854443
H	3.512811	-0.073906	-4.740277
C	-0.401017	1.679198	-0.325499
C	-2.223786	3.525389	-2.302862
H	-1.619662	2.661957	-2.604163
C	-3.311509	4.066656	0.030991
H	-2.864649	4.014811	1.029649
C	2.902403	2.296683	-1.197537
H	2.445539	1.445050	-1.724375
C	2.741571	3.149479	1.195476

H	2.568791	2.655773	2.160203
C	0.483868	0.919342	2.340659
C	-0.613848	1.729418	2.285207
C	1.051361	0.431823	3.657636
H	0.254735	-0.012149	4.265231
H	1.773627	-0.372546	3.479777
C	1.742491	1.534807	4.477243
H	2.694027	1.827095	4.026849
H	1.950408	1.184711	5.493596
H	1.119665	2.433163	4.543579
C	-1.482935	2.377939	3.352447
H	-1.086713	3.384836	3.553599
H	-2.474000	2.538897	2.906681
C	-1.684850	1.638513	4.675761
H	-1.979463	0.600765	4.501766
H	-2.482586	2.123905	5.246217
H	-0.788930	1.638864	5.299830
C	-1.454168	2.589399	-0.227106
C	-0.934291	2.064833	0.909657
N	-2.324602	3.387115	-0.834404
N	2.501123	2.110832	0.197156
C	1.761505	4.340054	1.183269
H	1.919518	4.998120	0.324347
H	0.723563	3.996071	1.161534
H	1.897102	4.941918	2.090279
C	4.177340	3.688551	1.241512
H	4.326514	4.267578	2.159841
H	4.908352	2.875501	1.217938
H	4.380299	4.357782	0.398555
C	2.339116	3.548715	-1.882955
H	2.500747	3.494091	-2.966511
H	1.263829	3.634165	-1.693967
H	2.831722	4.459790	-1.526294
C	4.411069	2.182428	-1.471501
H	4.941035	3.113464	-1.250709
H	4.846908	1.379221	-0.871363
H	4.584019	1.949159	-2.529171
C	-3.571733	3.422023	-3.013149
H	-3.396792	3.378374	-4.092521
H	-4.113278	2.520571	-2.718977
H	-4.204678	4.293029	-2.820304
C	-1.466032	4.790889	-2.715067
H	-0.552495	4.905748	-2.125350
H	-1.184441	4.719354	-3.770188

H	-2.076382	5.689452	-2.592218
C	-4.638459	3.306494	0.084823
H	-4.458398	2.245093	0.286423
H	-5.263083	3.708912	0.888535
H	-5.196178	3.393982	-0.851041
C	-3.494365	5.546385	-0.295038
H	-3.979424	5.703592	-1.261864
H	-4.134475	5.996483	0.469450
H	-2.535768	6.071499	-0.292214

TS(INT10-->INT11)

Al	1.212483	0.918759	0.173558
P	-1.428303	-1.136645	0.354393
Si	-3.812406	-2.134038	0.166894
N	1.937826	-0.840554	-0.002933
N	-2.450608	-1.852353	-0.877391
C	-0.050023	-2.218064	0.668452
C	1.291654	-1.965403	0.433203
C	2.040947	-3.219324	0.903969
H	3.052648	-3.332237	0.512853
C	1.949168	-3.189705	2.462069
H	2.613897	-3.948142	2.887853
H	2.242861	-2.220919	2.872480
C	0.455277	-3.516061	2.734867
H	0.346825	-4.470772	3.261097
H	-0.028843	-2.742387	3.327732
C	-0.133363	-3.607240	1.300955
H	-1.120369	-4.074440	1.245582
C	1.027295	-4.330776	0.595747
H	1.294242	-5.282550	1.070001
H	0.864267	-4.493855	-0.470362
C	-4.417822	-3.897517	0.383056
H	-4.877739	-4.279407	-0.535824
H	-5.175849	-3.946241	1.173218
H	-3.595016	-4.563549	0.658966
C	-5.271595	-1.033079	-0.274722
H	-4.900860	-0.015108	-0.442896
H	-6.051975	-0.999767	0.493429
H	-5.738280	-1.380643	-1.204591
N	-2.751341	-1.541004	1.433824
C	-3.126188	-0.854017	2.677473
C	-1.944832	-0.835474	3.647216
H	-1.680807	-1.857387	3.929088

H	-2.208517	-0.286665	4.558219
H	-1.069690	-0.352181	3.195221
C	-3.606600	0.579939	2.413102
H	-2.810241	1.168182	1.947447
H	-3.899231	1.073991	3.347207
H	-4.471751	0.580472	1.741947
C	-4.267842	-1.659668	3.309779
H	-5.159224	-1.655083	2.669702
H	-4.553424	-1.226322	4.273767
H	-3.958193	-2.697347	3.468586
C	-2.100029	-2.401669	-2.188333
C	-0.941123	-1.604425	-2.782539
H	-1.189348	-0.546201	-2.901741
H	-0.649541	-2.012175	-3.756883
H	-0.082984	-1.672486	-2.109469
C	-3.332368	-2.312166	-3.095870
H	-4.161990	-2.903334	-2.686500
H	-3.104109	-2.710180	-4.090218
H	-3.672158	-1.277046	-3.202955
C	-1.683110	-3.873637	-2.063805
H	-0.826108	-3.957004	-1.392430
H	-1.406281	-4.290037	-3.039405
H	-2.502915	-4.473981	-1.653955
C	3.318493	-0.998659	-0.404413
C	4.362049	-0.771407	0.514428
C	5.687039	-0.944871	0.104445
H	6.488155	-0.764526	0.816443
C	5.996290	-1.340280	-1.187790
H	7.030333	-1.476297	-1.489188
C	4.966521	-1.548818	-2.095140
H	5.204261	-1.844498	-3.112881
C	3.630685	-1.373002	-1.731670
C	4.106024	-0.317326	1.936853
H	3.029464	-0.393116	2.114039
C	4.821178	-1.196859	2.968981
H	4.627314	-2.259795	2.795346
H	4.481511	-0.944432	3.979710
H	5.905262	-1.043012	2.939633
C	4.514967	1.151450	2.102764
H	4.385581	1.480374	3.140052
H	3.914240	1.791906	1.446887
H	5.569240	1.286779	1.833622
C	2.549570	-1.610330	-2.769183
H	1.666558	-1.063428	-2.432825

C	2.198457	-3.099920	-2.842236
H	1.412933	-3.285705	-3.583257
H	1.849061	-3.466217	-1.873917
H	3.082087	-3.683480	-3.125725
C	2.906983	-1.087165	-4.163847
H	3.246067	-0.047002	-4.132349
H	2.024893	-1.139495	-4.811134
H	3.692049	-1.686825	-4.636886
C	-0.742157	0.988941	-0.435832
C	-3.115516	1.499789	-2.517560
H	-2.877021	0.453345	-2.295601
C	-3.675008	3.408185	-0.804628
H	-3.206179	3.656517	0.153269
C	2.765683	1.938197	-1.982076
H	2.420813	0.922286	-2.219034
C	2.289731	3.555152	-0.082863
H	2.097415	3.424538	0.988552
C	0.651914	1.611355	2.025169
C	-0.493102	2.329469	1.816510
C	1.375528	1.673588	3.356050
H	0.674137	1.406818	4.157320
H	2.159868	0.911933	3.395869
C	2.012048	3.032472	3.685662
H	2.809433	3.276637	2.978649
H	2.450129	3.018645	4.689504
H	1.279377	3.844327	3.647348
C	-1.209204	3.357656	2.682281
H	-0.679483	4.317465	2.608568
H	-2.195420	3.533011	2.235171
C	-1.422059	3.003032	4.157588
H	-1.799405	1.981542	4.261564
H	-2.156631	3.682612	4.600469
H	-0.505375	3.085468	4.745167
C	-1.869457	1.868513	-0.524670
C	-1.086963	2.019607	0.535448
N	-2.997092	2.159254	-1.201420
N	2.246184	2.201715	-0.639706
C	1.178241	4.505983	-0.572115
H	1.359229	4.868360	-1.588184
H	0.207082	4.001203	-0.558268
H	1.119139	5.382564	0.085168
C	3.642916	4.272296	-0.179433
H	3.629289	5.165009	0.456357
H	4.463254	3.626720	0.147373

H	3.854245	4.605355	-1.201053
C	2.197379	2.831123	-3.093746
H	2.467648	2.426601	-4.076520
H	1.106192	2.887773	-3.027758
H	2.599719	3.848465	-3.039336
C	4.300987	1.889659	-2.086887
H	4.742797	2.889041	-2.125602
H	4.726699	1.351653	-1.234549
H	4.603001	1.365286	-3.001553
C	-4.526327	1.526771	-3.094052
H	-4.538905	0.910368	-3.998495
H	-5.260811	1.118259	-2.395390
H	-4.836457	2.534795	-3.385492
C	-2.089049	2.017816	-3.527610
H	-1.082701	1.987527	-3.098216
H	-2.096156	1.385339	-4.422142
H	-2.309287	3.044310	-3.836028
C	-5.169553	3.235355	-0.526463
H	-5.346173	2.345492	0.084868
H	-5.532514	4.108025	0.025713
H	-5.761182	3.156428	-1.440752
C	-3.395217	4.568637	-1.761279
H	-3.867876	4.412275	-2.735819
H	-3.797408	5.496839	-1.343296
H	-2.318726	4.694971	-1.911705

INT11

Al	1.110582	0.882017	0.239969
P	-1.455535	-1.136746	0.329133
Si	-3.905957	-1.880798	0.149910
N	1.962765	-0.851051	0.089869
N	-2.482769	-1.833423	-0.865566
C	-0.085457	-2.127540	0.763968
C	1.277256	-1.937912	0.491087
C	1.964580	-3.248425	0.885726
H	2.952016	-3.395244	0.448474
C	1.945091	-3.262001	2.442238
H	2.599738	-4.053979	2.818489
H	2.293359	-2.312537	2.857316
C	0.453212	-3.539974	2.769788
H	0.328300	-4.520526	3.241555
H	0.038306	-2.788596	3.438029
C	-0.208894	-3.530707	1.363671

H	-1.219751	-3.949579	1.342586
C	0.875590	-4.283597	0.570908
H	1.106331	-5.274485	0.978586
H	0.655814	-4.366088	-0.495333
C	-4.639051	-3.581089	0.449652
H	-5.070372	-3.983745	-0.474356
H	-5.442524	-3.542327	1.192179
H	-3.877034	-4.281836	0.804199
C	-5.254078	-0.686269	-0.364165
H	-4.829213	0.322168	-0.433149
H	-6.084894	-0.664664	0.349950
H	-5.665431	-0.956226	-1.343879
N	-2.810638	-1.261921	1.375177
C	-3.118292	-0.784221	2.737507
C	-1.845572	-0.666593	3.569363
H	-1.402169	-1.653790	3.707793
H	-2.088191	-0.262385	4.558188
H	-1.107959	-0.008196	3.100043
C	-3.861239	0.557564	2.705468
H	-3.244631	1.323801	2.231002
H	-4.112257	0.876796	3.723553
H	-4.795575	0.468687	2.139297
C	-4.032395	-1.833333	3.385410
H	-4.997878	-1.892656	2.866653
H	-4.237513	-1.566493	4.427075
H	-3.561173	-2.821419	3.359984
C	-2.169552	-2.535597	-2.118452
C	-0.875995	-1.981111	-2.710182
H	-0.917034	-0.892062	-2.816091
H	-0.680757	-2.427369	-3.691477
H	-0.041532	-2.227260	-2.048798
C	-3.332589	-2.327009	-3.094935
H	-4.271941	-2.705449	-2.671375
H	-3.146912	-2.875484	-4.024236
H	-3.467824	-1.269280	-3.337785
C	-2.009286	-4.041499	-1.866756
H	-1.272740	-4.215040	-1.079682
H	-1.677274	-4.555037	-2.776183
H	-2.957705	-4.489085	-1.552062
C	3.345717	-1.030870	-0.281303
C	4.370604	-0.736567	0.637958
C	5.702074	-0.932881	0.259380
H	6.491347	-0.702158	0.969777
C	6.034346	-1.403135	-1.001266

H	7.073712	-1.552144	-1.276835
C	5.020445	-1.667820	-1.911865
H	5.274515	-2.021559	-2.907296
C	3.678219	-1.481280	-1.579861
C	4.098141	-0.147990	2.008537
H	3.018504	-0.195132	2.187596
C	4.799876	-0.920798	3.131522
H	4.595002	-1.994289	3.072479
H	4.459411	-0.556251	4.106753
H	5.885926	-0.784009	3.092133
C	4.528904	1.326653	2.017161
H	4.431403	1.763998	3.016530
H	3.918798	1.908540	1.316078
H	5.577612	1.415791	1.710632
C	2.623455	-1.788773	-2.627481
H	1.692960	-1.323862	-2.292017
C	2.408941	-3.302583	-2.747417
H	1.619228	-3.532185	-3.471599
H	2.136569	-3.747904	-1.787804
H	3.331964	-3.786597	-3.087206
C	2.958006	-1.212567	-4.008864
H	3.227904	-0.154274	-3.954656
H	2.090108	-1.311942	-4.669940
H	3.788794	-1.749653	-4.479010
C	-0.860179	0.493028	-0.138372
C	-2.837748	1.370187	-2.575779
H	-2.738832	0.325475	-2.260981
C	-3.147600	3.492742	-1.065482
H	-2.537597	3.824524	-0.217031
C	2.676442	1.816445	-1.988604
H	2.417608	0.763310	-2.161525
C	1.815347	3.566334	-0.367717
H	1.531185	3.545130	0.689275
C	0.665801	1.675304	2.083248
C	-0.574768	2.214235	1.913169
C	1.514521	2.055828	3.283283
H	0.918769	1.907822	4.193058
H	2.349072	1.356699	3.383090
C	2.085384	3.480286	3.298841
H	2.760599	3.645921	2.453772
H	2.653556	3.659831	4.218474
H	1.293145	4.234187	3.241868
C	-1.281378	3.336520	2.667559
H	-0.770955	4.285160	2.452729

H	-2.287739	3.441036	2.242487
C	-1.423746	3.169709	4.184275
H	-1.786149	2.167327	4.433907
H	-2.141556	3.896769	4.576659
H	-0.478334	3.328082	4.707622
C	-1.885243	1.576562	-0.375925
C	-1.318412	1.653442	0.797688
N	-2.679895	2.119966	-1.323517
N	2.010113	2.162552	-0.733286
C	0.627225	4.252534	-1.072012
H	0.852052	4.542213	-2.103414
H	-0.228311	3.567714	-1.085991
H	0.333584	5.161005	-0.529736
C	3.063331	4.454149	-0.441429
H	2.857942	5.419396	0.036002
H	3.907640	3.986630	0.075632
H	3.366587	4.658665	-1.473486
C	2.192640	2.571031	-3.236162
H	2.619659	2.114415	-4.136977
H	1.103310	2.548285	-3.321542
H	2.512920	3.618023	-3.223602
C	4.214308	1.868912	-1.936406
H	4.587482	2.896984	-1.961316
H	4.587609	1.386859	-1.028748
H	4.643322	1.341738	-2.798144
C	-4.216738	1.513754	-3.218250
H	-4.273822	0.843101	-4.082092
H	-5.013608	1.239366	-2.522362
H	-4.408296	2.525234	-3.585217
C	-1.706152	1.655444	-3.565093
H	-0.744051	1.517232	-3.060702
H	-1.758179	0.961892	-4.412714
H	-1.752324	2.675850	-3.957790
C	-4.610392	3.523540	-0.615281
H	-4.764181	2.818081	0.207882
H	-4.875396	4.526204	-0.263969
H	-5.291201	3.262687	-1.430555
C	-2.872190	4.474416	-2.205778
H	-3.459968	4.254227	-3.100567
H	-3.143314	5.482397	-1.876132
H	-1.812779	4.477933	-2.473523

TS(INT11-->8)

Al	1.052445	1.112254	0.202381
P	-1.212215	-1.242344	0.260748
Si	-3.137551	-2.822892	-0.315489
N	2.134650	-0.485446	0.349712
N	-1.804444	-2.042840	-1.137154
C	0.236253	-2.009695	0.916808
C	1.565486	-1.621938	0.824008
C	2.376849	-2.729952	1.500959
H	3.439044	-2.737698	1.258776
C	2.076562	-2.570280	3.022012
H	2.777366	-3.169404	3.611022
H	2.177147	-1.527252	3.337396
C	0.621658	-3.099217	3.147364
H	0.594014	-4.042175	3.705183
H	-0.039482	-2.397945	3.655741
C	0.231397	-3.348263	1.662073
H	-0.675867	-3.941583	1.535702
C	1.544492	-3.973348	1.160324
H	1.851635	-4.858286	1.729956
H	1.530014	-4.210878	0.094920
C	-2.971568	-4.687555	-0.136276
H	-3.155581	-5.164429	-1.107367
H	-3.711924	-5.092286	0.562439
H	-1.977130	-4.990449	0.201335
C	-4.874678	-2.550583	-0.967757
H	-5.597175	-3.091193	-0.345192
H	-4.955049	-2.957873	-1.982413
H	-5.168834	-1.501056	-0.999323
N	-2.599534	-1.840048	1.042561
C	-3.140548	-1.642276	2.396700
C	-2.263106	-0.683539	3.201845
H	-1.206521	-0.956586	3.146847
H	-2.571742	-0.692612	4.252541
H	-2.364198	0.332242	2.822154
C	-4.547415	-1.042551	2.284126
H	-4.495900	-0.092669	1.741614
H	-4.971541	-0.861667	3.277887
H	-5.222866	-1.717830	1.745444
C	-3.213808	-3.000807	3.103951
H	-3.835705	-3.703158	2.536039
H	-3.656323	-2.892819	4.099791
H	-2.215217	-3.435393	3.211179
C	-1.120542	-2.326483	-2.405469
C	-0.286795	-1.113008	-2.824818

H	-0.913196	-0.217410	-2.888553
H	0.182478	-1.292691	-3.798268
H	0.509396	-0.902375	-2.099856
C	-2.194514	-2.599349	-3.463704
H	-2.791310	-3.480207	-3.192832
H	-1.727536	-2.805368	-4.432149
H	-2.866963	-1.743803	-3.572564
C	-0.229581	-3.569094	-2.279279
H	0.485935	-3.435276	-1.466023
H	0.322637	-3.751336	-3.208936
H	-0.834592	-4.456023	-2.059499
C	3.544232	-0.541605	0.053623
C	4.461660	0.217171	0.806357
C	5.821176	0.175787	0.481526
H	6.520657	0.763428	1.070140
C	6.293002	-0.592555	-0.569501
H	7.350703	-0.607216	-0.812932
C	5.390020	-1.352466	-1.299749
H	5.751358	-1.969717	-2.118415
C	4.026066	-1.351554	-1.006257
C	4.046389	1.093104	1.971474
H	2.964470	0.994284	2.100107
C	4.703552	0.637120	3.279823
H	4.496499	-0.419277	3.479291
H	4.325299	1.228473	4.121038
H	5.790994	0.765412	3.244686
C	4.377322	2.560028	1.667916
H	4.138312	3.208145	2.517441
H	3.812001	2.899698	0.792678
H	5.444585	2.678846	1.451535
C	3.138278	-2.269073	-1.833907
H	2.113988	-2.174700	-1.467910
C	3.568384	-3.736945	-1.684143
H	2.825926	-4.400070	-2.143970
H	3.688417	-4.026168	-0.636865
H	4.525156	-3.911830	-2.188476
C	3.140683	-1.903686	-3.324182
H	2.782064	-0.886675	-3.498463
H	2.494630	-2.592826	-3.880854
H	4.149856	-1.983115	-3.743308
C	-0.888103	0.452151	0.062544
C	-4.588077	1.179766	-1.243884
H	-4.672048	0.322633	-0.570800
C	-3.292086	3.410635	-0.903910

H	-2.279402	3.596066	-0.535468
C	2.458094	1.553917	-2.247870
H	2.412033	0.477043	-2.042552
C	1.328451	3.559098	-1.183560
H	1.037210	3.816350	-0.158326
C	0.483966	2.236831	1.840098
C	-0.864132	2.383439	1.782991
C	1.257782	3.108160	2.810651
H	0.679287	3.216331	3.738317
H	2.185405	2.611610	3.108085
C	1.598537	4.512415	2.293842
H	2.262195	4.469406	1.426073
H	2.101013	5.099136	3.070384
H	0.691069	5.048638	1.993840
C	-1.722301	3.425145	2.473942
H	-1.128662	3.974488	3.209872
H	-2.020544	4.169259	1.719726
C	-2.985994	2.882965	3.147604
H	-3.594849	2.300123	2.446231
H	-3.603199	3.703224	3.527859
H	-2.732729	2.232383	3.990025
C	-2.629104	1.289556	0.110306
C	-1.548045	1.474164	0.850167
N	-3.501312	1.967776	-0.630026
N	1.791315	2.175913	-1.103585
C	0.043561	3.763588	-2.011396
H	0.229304	3.824747	-3.087548
H	-0.637616	2.924136	-1.830621
H	-0.458610	4.693656	-1.712802
C	2.390565	4.585601	-1.591584
H	2.012587	5.601491	-1.427362
H	3.305990	4.456248	-1.005109
H	2.650683	4.500589	-2.652064
C	1.770454	1.745642	-3.607903
H	2.232775	1.091640	-4.357225
H	0.703982	1.507105	-3.550615
H	1.877316	2.772485	-3.973318
C	3.955286	1.878788	-2.379401
H	4.124943	2.888127	-2.766877
H	4.452930	1.789933	-1.409735
H	4.433137	1.172496	-3.070489
C	-5.948567	1.871245	-1.254024
H	-6.702896	1.148782	-1.582163
H	-6.221853	2.219300	-0.254023

H	-5.988435	2.718518	-1.943989
C	-4.191877	0.636933	-2.616655
H	-3.204086	0.171045	-2.537404
H	-4.909644	-0.123360	-2.945949
H	-4.158961	1.420447	-3.378121
C	-4.237909	4.315013	-0.105884
H	-4.300379	3.988711	0.936376
H	-3.854675	5.341084	-0.121382
H	-5.246980	4.333291	-0.525061
C	-3.306737	3.766410	-2.390302
H	-4.306025	3.675569	-2.826191
H	-2.989148	4.807500	-2.509169
H	-2.616631	3.136340	-2.956739

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P	-1.151756	-1.234914	-0.413965
Si	-3.246608	-2.722167	-0.648846
Al	1.121017	1.032319	-0.007538
N	2.234608	-0.532859	-0.061596
N	-2.083941	-2.280959	0.584231
N	-2.343424	-1.578188	-1.613717
N	-3.365486	2.334224	0.762488
N	1.247898	2.164638	-1.458697
C	0.366563	-1.944304	-0.941880
C	1.689836	-1.649202	-0.592764
C	2.503487	-2.882556	-0.983014
H	3.582002	-2.724415	-1.015776
C	2.070055	-4.065467	-0.066191
H	2.749161	-4.909810	-0.219610
H	2.109256	-3.803165	0.992403
C	0.631548	-4.397810	-0.549793
H	-0.113689	-4.330577	0.246474
H	0.579566	-5.405164	-0.979342
C	0.398448	-3.311369	-1.627787
H	-0.451391	-3.500959	-2.287941
C	1.785028	-3.264415	-2.292126
H	2.115705	-4.231558	-2.688585
H	1.857191	-2.495718	-3.067968
C	-3.156775	-4.511204	-1.211816
H	-3.642077	-4.643828	-2.185344
H	-3.668944	-5.170192	-0.501898
H	-2.118494	-4.845633	-1.297543
C	-5.043443	-2.323021	-0.296446

H	-5.181178	-1.252575	-0.127529
H	-5.390882	-2.857451	0.595516
H	-5.685673	-2.632632	-1.128223
C	-2.031824	-2.616931	2.014856
C	-2.410279	-4.095239	2.174515
H	-1.735474	-4.743146	1.606560
H	-3.435903	-4.275919	1.827434
H	-2.367135	-4.384249	3.229672
C	-0.625830	-2.392397	2.562711
H	-0.319133	-1.348394	2.431173
H	0.092450	-3.036057	2.044154
H	-0.595812	-2.629866	3.631946
C	-3.040752	-1.767014	2.797492
H	-3.001926	-2.010201	3.865832
H	-4.059178	-1.964701	2.441419
H	-2.844077	-0.701659	2.655664
C	-2.548774	-0.963335	-2.927121
C	-1.319551	-1.140463	-3.828827
H	-1.202296	-2.195091	-4.100379
H	-0.400278	-0.824558	-3.330102
H	-1.434642	-0.558414	-4.750459
C	-2.898328	0.514830	-2.723586
H	-3.068401	1.028208	-3.677142
H	-2.104294	1.037410	-2.180339
H	-3.810686	0.575749	-2.117958
C	-3.738096	-1.659415	-3.595827
H	-3.543936	-2.731683	-3.710930
H	-3.909501	-1.238630	-4.591775
H	-4.654593	-1.523286	-3.010664
C	3.567844	-0.556143	0.475684
C	3.783960	-1.096615	1.762829
C	5.062645	-1.041383	2.321961
H	5.225280	-1.450279	3.315300
C	6.118785	-0.459343	1.639103
H	7.106932	-0.416691	2.086901
C	5.900018	0.073391	0.375811
H	6.730920	0.529960	-0.150408
C	4.640180	0.040386	-0.227639
C	2.654930	-1.676517	2.593671
H	1.832177	-1.904523	1.916011
C	3.050674	-2.966077	3.323206
H	3.575613	-3.665273	2.665025
H	2.154806	-3.462467	3.713158
H	3.702564	-2.758193	4.178693

C	2.137373	-0.645263	3.605698
H	2.956733	-0.288483	4.241932
H	1.372350	-1.090715	4.252204
H	1.691288	0.216186	3.098069
C	4.467308	0.605232	-1.630452
H	3.468313	1.052998	-1.693162
C	4.557979	-0.514539	-2.675951
H	4.499464	-0.099945	-3.688522
H	3.747179	-1.238265	-2.563481
H	5.510517	-1.049114	-2.578582
C	5.488048	1.692716	-1.976151
H	5.499009	2.494961	-1.230354
H	5.241645	2.130660	-2.948525
H	6.502391	1.287951	-2.061898
C	-0.709594	0.293881	0.227863
C	-1.307714	1.187865	1.099013
C	-0.411554	2.043053	1.973347
C	0.906180	2.106322	1.657214
C	-1.031281	2.672856	3.207216
H	-0.482122	3.580160	3.481916
H	-2.064183	2.982562	3.019663
C	-1.023433	1.684227	4.379846
H	-1.575762	0.776179	4.112681
H	-1.485834	2.117144	5.272666
H	0.001357	1.389659	4.628569
C	1.872002	2.966224	2.440884
H	1.644703	2.944848	3.516627
H	1.730431	4.014446	2.130284
C	3.341834	2.590735	2.237438
H	3.550022	1.575688	2.589912
H	4.003669	3.277605	2.774554
H	3.617418	2.621595	1.176178
C	-2.707870	1.345503	1.281668
C	-4.793174	2.519477	1.158702
H	-5.152703	3.405782	0.630352
C	-5.612384	1.309640	0.735363
H	-5.538140	1.142310	-0.344244
H	-6.665430	1.450268	0.995655
H	-5.230985	0.425708	1.255272
C	-4.888001	2.763503	2.661337
H	-5.933467	2.888859	2.958392
H	-4.335743	3.662174	2.953535
H	-4.466042	1.905919	3.195082
C	-2.769822	3.381884	-0.128024

H	-1.810618	2.961340	-0.450618
C	-3.625862	3.652363	-1.364667
H	-3.955451	2.727973	-1.843539
H	-3.024185	4.211310	-2.088146
H	-4.503663	4.264566	-1.134972
C	-2.522505	4.671406	0.650315
H	-3.460053	5.067922	1.057995
H	-2.102682	5.426311	-0.021784
H	-1.815573	4.516724	1.468895
C	0.635309	1.746889	-2.716273
H	-0.002212	0.894752	-2.441910
C	1.621065	1.183236	-3.753621
H	2.371938	1.920859	-4.055032
H	1.091189	0.850556	-4.655024
H	2.141469	0.317868	-3.330612
C	-0.319464	2.751916	-3.374925
H	-1.082322	3.083975	-2.663616
H	-0.829898	2.274475	-4.219897
H	0.197222	3.636030	-3.759420
C	1.795435	3.509684	-1.285320
H	2.453274	3.446704	-0.405544
C	0.743727	4.572061	-0.915187
H	0.062080	4.785907	-1.745282
H	1.227754	5.514533	-0.630048
H	0.155763	4.214663	-0.062991
C	2.690021	4.020037	-2.421864
H	3.486944	3.305788	-2.637947
H	3.152246	4.970628	-2.133465
H	2.130876	4.195707	-3.345853

8 Triplet

P	-0.994875	-1.404892	-0.442555
Si	-3.065305	-2.916280	-0.655567
Al	1.123440	1.071187	-0.093296
N	2.304686	-0.454133	0.018243
N	-1.947228	-2.392384	0.588470
N	-2.108444	-1.854146	-1.666774
N	-3.624563	2.373434	0.741580
N	1.268872	2.115835	-1.605332
C	0.577986	-2.056309	-0.822546
C	1.862073	-1.642691	-0.432495
C	2.762923	-2.855791	-0.662953
H	3.831032	-2.635533	-0.655379

C	2.342935	-3.978490	0.333784
H	3.077885	-4.788208	0.293367
H	2.305218	-3.624089	1.364832
C	0.956724	-4.443487	-0.193186
H	0.161475	-4.356531	0.552047
H	0.990252	-5.485136	-0.532497
C	0.725731	-3.473444	-1.376381
H	-0.073052	-3.770260	-2.061097
C	2.143730	-3.396776	-1.967729
H	2.553275	-4.372126	-2.254746
H	2.214909	-2.697998	-2.806649
C	-2.948091	-4.741531	-1.068208
H	-3.414697	-4.964003	-2.034152
H	-3.460187	-5.346799	-0.311788
H	-1.901979	-5.061083	-1.107901
C	-4.867464	-2.457154	-0.439464
H	-4.980441	-1.370081	-0.445365
H	-5.269899	-2.840187	0.505339
H	-5.478324	-2.877571	-1.245668
C	-1.976395	-2.543632	2.048671
C	-2.351983	-3.995153	2.367519
H	-1.632858	-4.691731	1.924986
H	-3.349552	-4.234899	1.977033
H	-2.375950	-4.154776	3.450371
C	-0.607633	-2.225414	2.645204
H	-0.317820	-1.189892	2.429253
H	0.155457	-2.895592	2.235472
H	-0.633773	-2.351502	3.733155
C	-3.029880	-1.606858	2.655630
H	-3.053102	-1.700668	3.747556
H	-4.027353	-1.848899	2.270684
H	-2.805810	-0.570104	2.390436
C	-2.287793	-1.306501	-3.015342
C	-1.005119	-1.457289	-3.843170
H	-0.809194	-2.517212	-4.038586
H	-0.133892	-1.051828	-3.323794
H	-1.107964	-0.941055	-4.804359
C	-2.730230	0.156996	-2.899322
H	-2.879249	0.610969	-3.885631
H	-1.992996	0.749835	-2.348325
H	-3.671599	0.204247	-2.338175
C	-3.398323	-2.106744	-3.702882
H	-3.135151	-3.169292	-3.752850
H	-3.543106	-1.745249	-4.725763

H	-4.350828	-1.998074	-3.172025
C	3.608835	-0.343266	0.614676
C	3.793477	-0.761143	1.950917
C	5.036677	-0.567804	2.557836
H	5.178233	-0.881006	3.588404
C	6.082301	0.033115	1.874990
H	7.041042	0.184664	2.361358
C	5.891859	0.444711	0.562505
H	6.714103	0.917498	0.037107
C	4.669430	0.270257	-0.090854
C	2.667299	-1.353540	2.779124
H	1.893908	-1.695175	2.090234
C	3.118610	-2.550351	3.625802
H	3.720181	-3.258723	3.047939
H	2.243058	-3.078833	4.019845
H	3.715052	-2.228783	4.486388
C	2.030645	-0.289349	3.684122
H	2.792318	0.177745	4.320340
H	1.274928	-0.743276	4.335777
H	1.543341	0.493447	3.093684
C	4.522182	0.703190	-1.542795
H	3.508891	1.100861	-1.676261
C	4.690387	-0.498130	-2.482832
H	4.664027	-0.172757	-3.528731
H	3.895051	-1.233529	-2.340875
H	5.652372	-0.992784	-2.302681
C	5.507548	1.800435	-1.952293
H	5.463075	2.661795	-1.277146
H	5.270139	2.144480	-2.963910
H	6.539820	1.433744	-1.976615
C	-0.665703	0.207500	0.096123
C	-1.449191	1.170616	0.798178
C	-0.630812	2.139560	1.655428
C	0.711229	2.214547	1.467706
C	-1.340563	2.839840	2.796051
H	-0.839757	3.788479	3.019188
H	-2.369762	3.081497	2.530381
C	-1.348711	1.955057	4.050185
H	-1.822610	0.990177	3.835321
H	-1.897070	2.427394	4.872365
H	-0.327822	1.748763	4.388649
C	1.570743	3.154903	2.288927
H	1.287113	3.128816	3.351290
H	1.373584	4.187967	1.959036

C	3.073578	2.887484	2.179214
H	3.335663	1.896254	2.561751
H	3.649777	3.629157	2.741972
H	3.411991	2.925297	1.136619
C	-2.805383	1.299022	0.602774
C	-4.978034	2.204948	1.290696
H	-5.552873	3.077800	0.965259
C	-5.664223	0.950804	0.755232
H	-5.633132	0.925746	-0.339078
H	-6.708360	0.920505	1.081028
H	-5.157022	0.059220	1.135841
C	-4.929932	2.190834	2.819036
H	-5.929422	2.029378	3.235266
H	-4.537265	3.133738	3.210900
H	-4.277886	1.378837	3.162685
C	-3.343716	3.537865	-0.130359
H	-2.276352	3.462037	-0.362916
C	-4.131266	3.459680	-1.438547
H	-3.915843	2.519840	-1.955240
H	-3.855454	4.288903	-2.097741
H	-5.210688	3.520735	-1.256694
C	-3.575702	4.860256	0.597657
H	-4.631653	5.010698	0.847009
H	-3.270842	5.686581	-0.051782
H	-2.987478	4.913499	1.517140
C	0.696848	1.631695	-2.857112
H	0.124228	0.738096	-2.572065
C	1.727305	1.131350	-3.883525
H	2.398287	1.928367	-4.218401
H	1.225894	0.718025	-4.767701
H	2.335072	0.336590	-3.438579
C	-0.326787	2.557408	-3.528507
H	-1.104787	2.854869	-2.816457
H	-0.807802	2.033064	-4.362751
H	0.133689	3.463854	-3.932856
C	1.718768	3.502110	-1.463334
H	2.342970	3.511242	-0.558104
C	0.598785	4.522187	-1.179019
H	-0.025628	4.711583	-2.056996
H	1.031677	5.481263	-0.868459
H	-0.036651	4.152516	-0.367295
C	2.625517	4.019802	-2.587082
H	3.466715	3.342802	-2.751951
H	3.024568	5.004726	-2.320232

H	2.086942	4.131306	-3.533500

mod-1

P	-1.590101	-0.008933	-0.047570
Si	-4.136221	0.237778	-0.056819
N	1.406851	-0.175830	0.034442
N	-2.817333	0.255546	-1.215052
N	-2.863440	-0.093139	1.097512
C	0.724853	-1.313934	-0.173917
C	-5.385995	-1.143902	-0.230132
H	-6.007869	-1.223003	0.668824
H	-6.057172	-0.973428	-1.078484
H	-4.879310	-2.101528	-0.381296
C	-5.003045	1.886823	0.104980
H	-4.272320	2.685845	0.261261
H	-5.575838	2.118709	-0.800127
H	-5.704369	1.894113	0.945870
C	-2.575248	1.006461	-2.435484
C	-2.768241	-0.714573	2.400826
C	2.831261	-0.160210	-0.041511
C	3.461633	-0.278755	-1.290698
C	4.855359	-0.248319	-1.340898
H	5.351612	-0.341770	-2.303174
C	5.606538	-0.084475	-0.181853
H	6.690430	-0.058678	-0.235355
C	4.965836	0.058298	1.043996
H	5.549607	0.196408	1.950060
C	3.573687	0.026657	1.133930
C	2.637592	-0.411967	-2.544862
H	1.878157	0.376968	-2.594178
C	2.874072	0.196015	2.457066
H	2.300886	1.130541	2.480737
C	0.646277	3.181376	-0.474365
C	0.639349	3.117485	0.884025
Al	0.355565	1.412643	0.125809
C	0.846528	4.197227	1.905731
H	-0.025390	4.279464	2.563569
H	1.701552	3.960361	2.548819
C	0.861794	4.353089	-1.386728
H	1.002260	5.296660	-0.843769
H	1.743037	4.190878	-2.016589
C	-0.664303	-1.458791	-0.228482
C	1.306869	-2.711831	-0.286976

H	2.358939	-2.760302	-0.570615
C	0.972057	-3.404455	1.069392
H	1.500728	-4.359937	1.130860
H	1.287124	-2.796064	1.921427
C	-0.569587	-3.609988	1.003042
H	-0.822830	-4.675515	1.000900
H	-1.091471	-3.140795	1.840233
C	-0.940864	-2.947894	-0.352111
H	-1.930115	-3.209096	-0.733744
C	0.267414	-3.376919	-1.211637
H	0.398175	-4.463291	-1.271025
H	0.244485	-2.947033	-2.216648
H	1.026668	5.181406	1.454536
H	0.011007	4.476659	-2.066146
H	-2.269245	2.043107	-2.240520
H	-3.483824	1.019624	-3.043995
H	-1.788712	0.525747	-3.027162
H	3.270726	-0.340522	-3.432606
H	2.106775	-1.370705	-2.587247
H	3.595735	0.214013	3.277628
H	2.162200	-0.616280	2.638236
H	-3.404812	-0.193115	3.122017
H	-3.058127	-1.774040	2.382661
H	-1.737992	-0.655212	2.770227

mod-2

N	2.839811	-5.261502	-5.043322
N	4.479495	-5.509245	-3.734309
C	3.180636	-5.083654	-3.731688
C	3.870475	-5.769698	-5.817458
C	4.920535	-5.928372	-4.979164
C	1.523360	-4.944114	-5.556567
H	0.935677	-4.567120	-4.720547
C	5.300405	-5.514629	-2.541309
H	4.685183	-5.133812	-1.727122
H	3.770003	-5.969897	-6.873633
H	5.920489	-6.294682	-5.156888
H	1.583924	-4.178228	-6.335469
H	1.041643	-5.835456	-5.969347
H	6.176294	-4.871631	-2.669061
H	5.634154	-6.529030	-2.303532

mod-INT1

P	-1.811410	0.252826	0.118196
Si	-4.279151	-0.360270	-0.209486
N	1.068500	0.773481	0.336188
N	-3.177168	-0.077300	1.114102
N	-2.907559	0.045680	-1.221722
N	0.923681	-2.049990	-2.344531
N	2.589805	-2.276445	-1.023877
C	0.268810	1.834687	0.353654
C	-5.716370	0.830038	-0.389427
H	-6.209655	0.713447	-1.361102
H	-6.472129	0.659538	0.384649
H	-5.368300	1.863901	-0.302292
C	-4.875237	-2.131675	-0.303832
H	-4.014676	-2.807569	-0.270149
H	-5.528771	-2.371547	0.542692
H	-5.438330	-2.330245	-1.221691
C	-3.064822	-0.629584	2.455126
C	-2.794197	0.798231	-2.452324
C	2.476745	0.944084	0.325213
C	3.175814	1.013169	1.547526
C	4.567165	1.088234	1.527140
H	5.106923	1.139486	2.469134
C	5.266602	1.105405	0.321568
H	6.350742	1.165904	0.320721
C	4.567983	1.057032	-0.878351
H	5.105972	1.084877	-1.823459
C	3.171417	0.977218	-0.896211
C	2.407742	1.026105	2.842327
H	1.718180	0.177430	2.888324
C	2.450494	0.930681	-2.222050
H	1.366356	0.903015	-2.084898
C	1.322228	-1.810017	-1.075596
C	1.927111	-2.644887	-3.081488
C	2.982755	-2.788606	-2.242508
C	-0.380253	-1.685475	-2.876364
H	-1.088060	-1.565374	-2.052376
C	3.439829	-2.253212	0.163304
H	2.809104	-2.044426	1.029691
C	0.420228	-2.023617	2.172651
C	-0.443016	-2.714117	1.377711
Al	0.224426	-1.082548	0.521978
C	-1.177804	-3.985475	1.715413
H	-2.263256	-3.843368	1.624163

H	-0.921125	-4.781433	1.005403
C	0.854288	-2.317082	3.586871
H	0.487753	-3.282312	3.961659
H	1.948723	-2.319953	3.678345
C	-1.135767	1.829017	0.264782
C	0.681593	3.295518	0.431808
H	1.694723	3.472813	0.797382
C	0.384071	3.906803	-0.969879
H	0.818193	4.908981	-1.034273
H	0.819049	3.305879	-1.773484
C	-1.171817	3.956918	-1.024037
H	-1.526681	4.992849	-1.064589
H	-1.581153	3.428123	-1.887787
C	-1.577375	3.282748	0.313842
H	-2.616176	3.445075	0.609568
C	-0.496191	3.865662	1.250370
H	-0.488807	4.961568	1.284205
H	-0.550514	3.459147	2.263712
H	1.797675	-2.918751	-4.116751
H	3.960436	-3.217334	-2.397090
H	-0.310603	-0.748782	-3.437114
H	-0.734291	-2.479406	-3.536960
H	4.203120	-1.477144	0.062343
H	3.905591	-3.233705	0.282252
H	-0.978715	-4.365464	2.728206
H	0.495447	-1.539530	4.274172
H	-2.904394	-1.714400	2.456405
H	-3.970115	-0.399420	3.025932
H	-2.217699	-0.171008	2.975585
H	3.085747	0.991630	3.699215
H	1.800423	1.936530	2.924645
H	2.748882	0.045689	-2.798608
H	2.698489	1.810128	-2.826872
H	-3.071170	0.184769	-3.318182
H	-3.421410	1.701958	-2.458626
H	-1.756743	1.128125	-2.592498

mod-7

C	-2.910721	-1.418156	-0.928249
C	-1.622387	-1.019789	-0.982514
C	-2.337280	-1.157633	-2.187533
N	-4.034704	-1.782606	-0.290249
N	-0.443699	-0.671335	-0.441167

C	-5.149408	-2.257816	-1.088536
H	-4.987490	-1.947030	-2.121445
C	-4.045818	-2.111255	1.117223
H	-3.235434	-1.581155	1.620144
C	-0.141346	-0.907071	0.952504
H	-1.067143	-0.905818	1.530105
C	0.680336	-0.458837	-1.334039
H	1.242835	0.429151	-1.026086
H	-4.995756	-1.797609	1.563195
H	-3.924480	-3.190491	1.288262
H	-6.087013	-1.828191	-0.719528
H	-5.228763	-3.352944	-1.052184
H	0.505139	-0.108054	1.330863
H	0.371846	-1.867278	1.105556
H	1.360762	-1.321391	-1.332677
H	0.292855	-0.313260	-2.343181

mod-INT6

Al	1.348127	1.475609	0.528187
P	-1.364142	-0.474231	0.705980
Si	-3.757348	-1.438134	0.959570
N	1.757282	-0.208128	-0.229686
N	-2.982297	-0.228106	-0.035131
C	-0.452592	-1.283783	-0.582029
C	0.914089	-1.143117	-0.739475
C	1.378660	-2.318766	-1.595540
H	2.358440	-2.199216	-2.060748
C	1.243074	-3.600448	-0.721644
H	1.671789	-4.451610	-1.259686
H	1.780820	-3.507092	0.224520
C	-0.296353	-3.757763	-0.552507
H	-0.643824	-4.704989	-0.980583
H	-0.622043	-3.714715	0.489548
C	-0.843415	-2.542160	-1.350390
H	-1.902184	-2.614376	-1.615722
C	0.156753	-2.484896	-2.518335
H	0.197906	-3.405991	-3.111864
H	-0.003706	-1.624695	-3.176005
C	-4.585955	-2.817805	-0.010271
H	-5.470251	-2.457823	-0.548834
H	-4.922597	-3.604865	0.673781
H	-3.902440	-3.272868	-0.732624
C	-4.994866	-0.810179	2.226654

H	-4.579320	0.031225	2.790228
H	-5.264245	-1.594583	2.943437
H	-5.922268	-0.477114	1.747484
N	-2.183890	-1.717267	1.634010
C	-1.713474	-2.131497	2.940502
C	-3.179881	-0.007888	-1.452605
C	3.134819	-0.583560	-0.102861
C	3.539596	-1.262726	1.057218
C	4.880034	-1.630361	1.183712
H	5.200846	-2.161046	2.076353
C	5.802917	-1.312488	0.192999
H	6.843215	-1.602180	0.305168
C	5.393280	-0.611027	-0.936296
H	6.114723	-0.347362	-1.705283
C	4.059889	-0.233479	-1.096366
C	2.547669	-1.527121	2.161969
H	1.622213	-1.980891	1.788826
C	3.605384	0.543899	-2.302076
H	2.838496	-0.003900	-2.863803
C	-0.210818	2.148177	-0.546974
C	-0.005916	1.519044	-3.680981
H	-0.391592	0.618635	-4.172957
C	-2.286335	2.501642	-3.728022
H	-2.966456	3.084715	-3.105731
C	-3.839775	3.103096	0.045395
H	-3.900055	3.353054	-1.015286
C	-2.197336	2.789026	1.867783
H	-2.749058	1.912273	2.226664
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C	1.784122	2.216404	2.216495
C	3.915893	3.446886	1.410882
H	4.793553	2.872788	1.091108
H	3.873019	4.332476	0.766251
C	1.791228	2.496240	3.695009
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H	0.860939	2.987040	4.007293
C	-0.999565	2.337079	-1.663217
C	-1.509273	2.616916	-0.413755
N	-1.084983	2.196529	-2.978297
N	-2.449772	2.972384	0.440968
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H	-2.556209	-2.316109	3.616980
H	-1.119068	-3.052414	2.887587
H	-3.924100	-0.702686	-1.866416

H	-3.533472	1.011358	-1.671934
H	-2.242659	-0.162577	-2.008800
H	-4.368852	2.159679	0.232514
H	-4.306165	3.906310	0.622957
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H	4.442377	0.747533	-2.975108
H	2.260995	-0.582544	2.641202
H	2.977937	-2.185579	2.921454
H	1.849615	1.561794	4.266375
H	4.092382	3.788078	2.440077
H	-2.528463	3.679716	2.410567
H	-1.128597	2.626593	2.030709

References

S1 R. L. Falconer, G. S. Nichol, M. J. Cowley, *Inorg. Chem.* **2019**, *58*, 17, 11439–11448.

S2 SAINT, Program for data reduction, Bruker-AXS.

S3 SADABS, Program for data correction, Bruker-AXS.

S4 SHELXT, G. M. Sheldrick, *Acta Crystallogr. Sect. A,* **2015**, *71*, 3-8.

S5 SHELXL, G. M. Sheldrick, *Acta Crystallogr. Sect. C*, **2015**, *71*, 3-8.

S6 Spek, A. L., *Acta Cryst.* **2015**, C71, 9-18.

S7 Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

S8 Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215.

S9 F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys*., **2005**, *7*, 3297.